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5th Vienna Symposium on Mathematical Modelling

February 8-10, 2006
Vienna University of Technology, Austria

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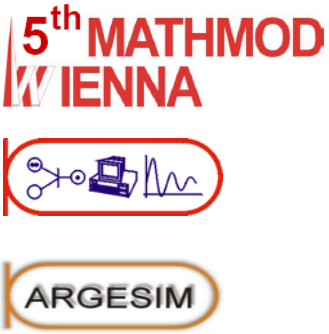
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I. Troch, F. Breitenecker (Eds).

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Series Editor:
Felix Breitenecker (ARGESIM / ASIM)
Div. Mathematical Modelling and Simulation, Vienna University of Technology
Wiedner Hauptstrasse 8 - 10, 1040 Vienna, Austria
Tel: +43-1-58801-10115, Fax: +43-1-58801-10199
Email: Felix.Breitenecker@tuwien.ac.at

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Editors: Inge Troch, Felix Breitenecker
Div. Mathematical Modelling and Simulation,
Vienna University of Technology
Wiedner Hauptstrasse 8 - 10, 1040 Vienna, Austria
Email: Inge.Troch@tuwien.ac.at

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ARGE Simualtion News (ARGESIM)
c/o F. Breitenecker, Div. Mathematical Modelling and Simulation, Vienna Univ. of Technology Wiedner Hauptstrasse 8-10, A-1040 Vienna, Austria
Tel.: +43-1-58801-10115, Fax: +43-1-58801-42098
Email: info@argesim.org; WWW: http://www.argesim.org

Proceedings
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Abstract Volume

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Content

Content

Preface

Improvement of existing systems, design of new systems, strategies, controls etc. and the cost for doing so depend to a great extent on appropriate modelling of the system or of the task in question. Especially, modelling of the dynamic and static properties of a system to be constructed, to be improved or to be influenced is today considered as standard pre-requisite to derive an appropriate solution. However, also relevant background information connected with this task has to be modelled, such as restrictions on controls or on systems' behaviour, wanted and/or unwanted smoothness properties of solutions, available devices and their relevant properties, restrictions imposed e.g. by law. Normally, it will not be possible to describe all details of a system's behaviour or all requests imposed on the solution by traditional mathematical expressions. Further, there is the additional request that the resulting mathematical model should be an accurate description of the task with parameters which can be determined with reasonable cost and within sufficiently short time and, should at the same time be a model which is sufficiently easy to handle.

Therefore, the decision which effects or requirements are to be included in a model and which can be neglected is a difficult decision and normally modelling is to be done in several steps and requires simplification but also inclusion of more details for some parts of the model until a model is established which is at the same time accurate enough for the task in question and which can be handled by men and/or computers with sufficient ease.

The invited lectures reflect this wide spectrum of important topics of current interest ranging from applications, over methodological and theoretic aspects to questions how to handle uncertainties of various types:

- Gerta Zimmer (Siemens Power Generation, Germany):
  Modeling and Simulation of Steam Turbine Processes; Individual Models for Individual Tasks
- Leon Zlajpah (Jozef Stefan Institute, Ljubljana, Slovenia):
  Simulation in Robotics
- Peter Schwarz (Fraunhofer EAS, Dresden, Germany):
  Simulation of Systems with Dynamically Varying Model Structure
- Rudolf Rabenstein, Stefan Petrausch (University Erlangen-Nuremberg, Germany): Block-Based Physical Modeling
- Kurt Schlacher (University of Linz, Austria): Mathematical Modeling for Nonlinear Control, A Hamiltonian Approach
- Reinhard Viertl (Vienna University of Technology, Austria):
  Fuzzy Models for Precision Measurements
- Siegfried Tagesen (University of Vienna, Austria):
  Dependent Nuclear Reaction Probabilities from Pointwise Measurements Including Full Covariance Information

Further, it is not astonishing that there will many presentations during the 5th MATHMOD conference which are concerned with the modelling of a concrete system or subsystem for a specific task. Examples are to be found in the sessions on 'Physical Modelling', on the modelling of 'Electrical and Power Systems', of 'Mechanical Systems', of 'Economic Systems' and on 'Modelling in Biology and Physiology', but also in the sessions on

'Modelling for/and Control' and on 'Process Modelling'. These sessions were compiled from papers selected for presentation after a reviewing process which was based on extended abstracts.

Moreover, also the so-called 'special sessions' reflect the large variety of topics which are of interest for many researchers but also for many people working in industries or other application-oriented institutions. These sessions have been organized by colleagues from many countries to serve a twofold purpose: There, people interested in a rather specific type of systems or in more theoretic questions, in modelling approaches or methods can meet, present results and discuss issues of common interest. But, at the same time, these sessions were put together to allow each participant working in a different area a look over the fence of his own garden and to see what are topics of actual interest in other disciplines or, in which way problems analogue to their owns are treated there. Therefore, some of these organized sessions will start with a short survey lecture on the respective state-of-the art and continue with more specific topics. Thus, the organizers hope that many participants will get with some ease a good overview on what is going on in other fields of applications or in theory and will find at the same time in such sessions ideas which help them directly or after some adoption to solve their own problems.

Consequently, there are special sessions devoted to applications and others dealing more theoretical or methodological aspects as it is the case also for the sessions compiled from submitted and reviewed papers. One group of organized sessions is concerned the modelling of systems of a rather specific nature. Among them we find application areas where mathematical models have a very long tradition as e.g. in mechanical, electrical and other engineering sciences or, areas where models are used since several decades with growing success as e.g. for biological, bio-technical, chemical and environmental systems or, modelling topics important for and in industrial systems, reflected in organized sessions such as 'Optimization in multibody dynamical models' (F.L.Chernousko, N. N. Bolotnik), 'Control-oriented modelling of advanced multi-link manipulators' (P. Rentrop, R. Callies), 'Nonlinear Oscillations' (A.Steindl, H.Ecker), 'Structural control' (H..Irschik, M.Gusenbauer), 'Object-oriented modelling in mechatronics' (G..Ferrett, F. Casella), 'Multiscale Modelling in Materials Science' (M. Burger, P.Weinberger), 'Mathematical Modelling of Semiconductor Devices' (M. Burger, H. Kosina), 'Modelling and Simulation for Control System Design, Coordination and Supervision' (B..Zupancic), 'Modeling and Simulation in the Pulp and Paper Industry' (B. Lie), 'Rule-based Automation of Engineering in Process Industries' (U. Epple, R. Jorewitz), 'Advanced mathematical methods for simulation based research services' (K. Juslin), 'Mathematical models of co-operative multiagent systems' (D. Matko), 'Future Mobile Communication Systems' (C. Überhuber), 'Modelling and Simulation in Systems Biology' (W. Wiechert), 'Modelling of Environmental Systems' (A. Gnauck, B. Luther), 'Efficient Operation of Sequential Batch Reactors for Wastewater Treatment' (D. Dochain), 'Mathematical modelling and control of chemical and bio-chemical processes' (P..Bogaerts, J.van Impe).

Some of the above sessions are concerned also with theoretical or numerical aspects, with modelling methodologies, with model reduction and simplification, with validation and model quality or, use models which are not the traditional differential equations or composed of models of various types. Aspects such as these are especially true for organized sessions such as 'Stochastic Optimization Methods' (K. Marti), 'Modeling of distributed-parameter systems for control purposes' (A. Kugi), 'Optimal Control of Applications described by DAEs/PDEs/PDAEs' (K. Chudej, R. Griesse), 'PDAE Models in Engineering Applications' (B. Simeon), 'Port-based modelling and control (on a geometric basis)' (P. Breedveld),

'Model Reduction and Reduced Order Modelling' (B. Lohmann, P.C. Müller), 'Issues of Model Quality and Validation' (D.Murray-Smith), 'Petrinets: Current Research Topics and their Application in Traffic Safety and Automation Engineering' (E. Schnieder, J. R. Müller), 'Tool Integration and Interchange Formats for Hybrid Systems' (M. Remelhe, S. Engell).

Thus, the various contributions reflect also the fact that today systems to be modelled can be of very different nature, they may be deterministic or stochastic, continuous or discrete or discrete-event or hybrid, lumped parameter or distributed parameter etc. Consequently, a wide variety of formal models is to be discussed and used demonstrating that the term 'mathematical model' includes classical models such as differential or difference equations, Markov processes, event systems as well as more special or more recent approaches such as Bond graphs, Petri nets, fuzzy models or neural nets.

Volume 1, the printed Abstract Volume, contains one-page abstracts of seven invited papers, of contributed papers and of posters. Volume 2, the Full Papers' Volume, on CD ROM, consists of the full text versions of the invited papers and of the contributed papers. Both volumes of these Proceedings start with the manuscripts of the invited lectures.

Then follow contributed papers which were either contributed upon invitation of a session organizer or, which were selected for presentation after a reviewing process which was based on extended abstracts. All these contributions were collected and arranged in sessions according to their main thematic point. Such a grouping is by no means easy because many contributions address several different aspects in a balanced manner. Therefore, the arrangement chosen for this volume follows rather closely the one of the conference where also time limitations had to be observed. The Abstract Volume contains as its last part the abstracts of the contributed posters, which were undergoing also a review procedure and which were on display during the whole conference and discussed during a special poster session.

The editors wish to express their sincere thanks to all who have assisted them by making the idea of this symposium known within the scientific community or by acting as sponsor or cosponsor, who have assisted them in the reviewing process and have done a good job by putting together special sessions devoted to one main theme. Last but not least the editors would like to thank the ARGESIM team for their support in the preparation of these Proceedings, especially our colleagues Gerhard Höfinger and Florian Judex.

Vienna, January 2006 I.Troch, F. Breitenecker

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5th MATHMOD Vienna

Plenary Lectures

MODELING AND SIMULATION OF STEAM TURBINE PROCESSES; INDIVIDUAL MODELS FOR INDIVIDUAL TASKS

G. Zimmer, Siemens AG, Germany

Corresponding Author: G. Zimmer,
Siemens AG, Power Generation, P11M3
Postbox 101755, D-45466 Mülheim, Germany
Phone: +49 208 456 3747, Fax: + 49 208 456 3363
email: gerta.zimmer@siemens.com

Abstract. This paper presents a brief overview of models which simulate the thermodynamic behaviour of a steam turbine with respect to transient operations. Three different approaches will be introduced and compared with respect to different operating situations.

1. Introduction

Today, steam turbine industry faces numerous challenges concerning efficiency, commissioning time, start-up times, operation, availability, safety, cost effectiveness, etc. Many of these tasks can be supported by simulating the transient operational behavior of the turbine in advance. For example the commissioning time can be shortened if the turbine controllers are initialized with well-tuned pre-set parameters, cost effectiveness can be increased by setting aside unnecessary devices and exactly determining material specifications, safety may be increased by predicting the impacts of failures and thus taking the necessary precautions.
Different tasks require different details regarding the employed turbine simulation model. Thus, the turbine controller may be well tuned with less complex simulation models of turbine, generator and electrical grid, whereas detailed studies of failures may require detailed modeling of the turbine-internal thermodynamic processes.

2. General set-up

The principal task in operating a steam turbine is to convert the energy of hot steam into electrical energy. Thus, hot steam with up to 300 bar and 600°C is condensed to approximately 0,03 bar and 25°C. The released energy is transform into rotational energy, which, in turn, drives a generator that finally delivers electrical energy.
In general, a steam turbine consists of three different expansion sections, with high-, intermediate-, and low-pressure. In order to increase the degree of efficiency, a re-heater is located between the high- and intermediate pressure section. At the entrance of the high- as well as at the intermediate-pressure section the admittance of steam may be controlled by appropriate control valves.

3. Different Simulation Models

In order to meet different needs, a couple of turbine models with different degrees of complexity were developed. The simplest of which describes the turbine as a linear system. An extension takes the thermodynamic originated nonlinearities into account but still abides the ideal-gas-behavior assumption. Finally, the most rigorous model thoroughly considers mass and energy flows as well as water-steam-properties in detail.
The three outlined approaches as well as their range of application will be exemplified by reference turbine models, each model built with a different level of detail. Different operating conditions and failures, respectively, will be considered and simulated with the varying models. The simulation results will be compared to actual plant data.
It will be discussed, which level of detail is required for standard tasks as well as some necessary failure investigations.

4. Literature

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Block-Based Physical Modeling

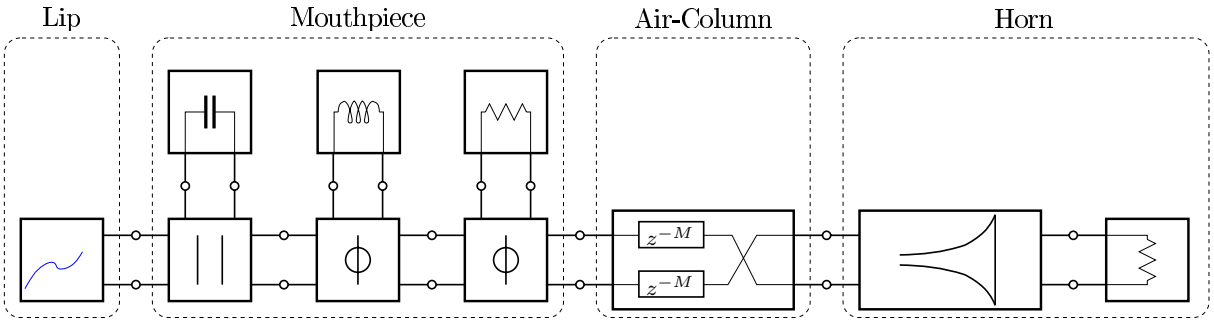
R. Rabenstein, S. Petrausch

Corresponding Author: R. Rabenstein
University Erlangen-Nürnberg
Telecommunications Laboratory
Cauerstraße 7, D-91058 Erlangen, Germany
Phone: +49 9131 8528717, Fax: +49 9131 8528849
email: rabe@LNT.de

Block-based physical modeling is a methodology for modeling physical systems with different subsystems. Each subsystem may be modeled according to a different paradigm. Connecting systems of diverse nature in the discrete-time domain requires a unified interconnection strategy. Such a strategy is provided by the well-known wave digital principle [1, 2], which has been introduced initially for the design of digital filters. The use of wave variables for the interconnection network avoids the formation of delay free loops and yields computable algorithms. This contribution describes the wave digital principle as a starting point for the more general idea of block-based physical modeling. It is shown how arbitrary discrete-time state space representations can communicate via wave variables. A series of examples explain how to combine linear and nonlinear blocks, lumped and distributed parameter systems, and how to model complex geometries from simpler blocks.

The strength of the modeling approach presented here is that it allows to generate real-time algorithms with low latency. Of course this is only possible if appropriate models are chosen for the individual blocks. However, by the example of musical instrument modeling it is demonstrated that an automated synthesis procedure of mixed models generates real-time algorithms which are playable by a musician.

A block-based physical model of a brass instrument is shown below. The lips are represented by a nonlinear model according to [3]. The resonating properties of the mouthpiece are modeled by the wave digital equivalence of a corresponding electrical circuit. The air-column model is a dual delay line which represents the propagation of acoustic waves. For the horn, the functional transformation method is used. These modeling blocks and the underlying methods are discussed in the paper, along with other examples for musical instrument and room acoustic modeling.



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FUZZY MODELS FOR PRECISION MEASUREMENTS

Reinhard Viertl

Department of Statistics and Probability Theory
Vienna University of Technology
Wiedner Hauptstraße 8-10, 1040 Wien, Austria
Phone: +43 1 58801-10720
email: R.Viertl@tuwien.ac.at

Fuzzy models are standard to describe linguistic variables and other qualitative information. Moreover they were used successfully in fuzzy control. For the description of measurement results fuzzy models are not used presently.

The measurement of continuous quantities is basic for all systems in engineering and natural sciences. This concerns one-dimensional quantities as well as vector quantities. Presently statistical models are used to analyze measurement uncertainty, and sometimes interval mathematics.

Statistical models are suitable to model variation and errors, but not to describe the imprecision of individual measurement results of continuous quantities.

Using intervals is a first step to describe measurement uncertainty. But this model is not sufficient. Since intervals are subsets of the set of real numbers, fuzzy subsets as generalizations of intervals and numbers are suitable to describe measurement results. Fuzzy subsets are characterized by their so-called membership functions.

All engineering and scientific measurements of continuous quantities are not precise numbers but more or less non-precise. This imprecision is different from variation and errors. Therefore statistical models are not suitable to describe the imprecision of individual measurement results.

So-called non-precise numbers, which are special fuzzy subsets of the real line but more general than fuzzy numbers and fuzzy intervals, are the best up to date model for one-dimensional measurement results. Non-precise numbers are characterized by so-called characterizing functions, which are specialized membership functions of subsets of the set of real numbers.

Of crucial importance are procedures to obtain the characterizing function of non-precise numbers. Methods how to obtain the characterizing function of a non-precise number as result of a measurement will be given in the contribution.

For vector-valued continuous quantities a suitable model to describe individual measurement results are so-called fuzzy vectors. These fuzzy vectors are special fuzzy subsets of the k-dimensional Euclidean space. The related membership functions are called vector-characterizing functions.

Methods for obtaining the vector-characterizing function of a fuzzy vector describing vector measurements will be discussed in the contribution.

Moreover results concerning statistical data analysis of non-precise measurements will be presented.

Reference

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MATHEMATICAL MODELING FOR NONLINEAR CONTROL A HAMILTONIAN APPROACH

K. Schlacher
Johannes Kepler University Linz, Austria

Institute of Automatic Control and Control Systems Technology
Altenbergerstraße 69, 4040 Linz, Austria
Phone: +43 732 2468 - 9731, Fax: + 43 732 2468 - 9734

email: kurt.schlacher@jku.at

Modeling is an essential, or the most important step for the analysis and design of dynamic systems. Especially, modern model based nonlinear control requires a good mathematical description of the system we want to control, for both, the system analysis and the controller design. Obviously, the term nonlinear system is too broad, and one is interested in subclasses of nonlinear systems with at least two properties. These classes should cover real world problems. There should exist controller design methods, powerful enough to admit a systematic design of the closed loop with certain properties. Now, classical Hamiltonian systems have a rich mathematical structure, which has been extended such that dissipative effects or inputs and outputs, or better ports, are included in this class.
One of the main purposes of mathematical models in control is the description of the process or plant to be controlled such that one can construct the controller. Now, control theory offers many analysis and design methods, which exploit both, the individual mathematical model, but even more important, the underlying mathematical structure of the model. Therefore, it makes sense to classify models according to their common structure. Linear and time invariant models, described by explicit ordinary differential equations, are an excellent example, for which a rich collection of design methods is available. Since this class was and is so successful in many applications, a further division does not seem to be necessary. This picture changes dramatically if we turn to nonlinear systems, where no general theory, comparable to the power of the linear one, is currently available. But for certain classes of nonlinear systems there exists already a rich theory for the controller design. Affine input systems form such a class or Lagrangian systems with inputs, whose origin lies in the calculus of variation. Classical Hamiltonian systems are closely connected to Lagrangian ones, but they are, like classical Lagrangian system, too poor to be of interest for control purposes because of the absence of inputs or dissipation. Today, these drawbacks are removed and a rich theory for lumped parameter Hamiltonian systems, which include inputs, outputs and dissipation, is available.
This contribution studies dynamic systems from a Hamiltonian point of view. If the system allows the dividing of the evolution of the Hamiltonian, which often corresponds to the energy of a physical system, into an internal flow, which preserves the Hamiltonian, into a dissipative flow, which causes a decrease of Hamiltonian, and into a flow caused by the inputs, then this property has a severe impact on the mathematical structure of the system equations. This fact has several advantages. The physical properties of a system are well reflected by the formal mathematical description and therefore, they can be exploited by suitable controller design methods. As a motivation for the Hamiltonian description, linear systems are studied first together with structure preserving controller design methods. Since also nonlinear lumped parameter systems, described by ordinary differential equations, exhibit these essential structural properties, certain controller design methods for the class of port controlled Hamiltonian systems like damping injection, PI-control or nonlinear H_2- or H_∞-control will be presented.
The Hamiltonian description is not limited to lumped parameter systems, but their extension to distributed parameter systems, described by partial differential equations, is not unique at all. After a short introduction into the required mathematical framework, a formulation for distributed Hamiltonian systems will be presented, which preserves the essential structural properties of the lumped parameter case. This fact allows us to adapt the already presented controller design methods for design problems like distributed damping injection, PI-control or H_2-, H_∞-control. But the presented methods are formal ones, i.e. they rely on the formal properties of the system equations only. Therefore, problems like the existence and uniqueness of solutions or the stability of the closed loop cannot be discussed within the presented theory. Finally, the contribution closes with an example, which is supposed to demonstrate the applicability of the presented approach to real world problems, where an elastic structure with piezoelectric material is modelled.

SIMULATION IN ROBOTICS

Leon Žlajpah

Jožef Stefan Institute
Jamova 39, 1000 Ljubljana, Slovenia
Phone: +386 1 4773 577 Fax: + 386 1 4773 154
leon.zlajpah@ijs.si

Simulation has been recognized as an important research tool since the beginning of the 20th century. In the beginning, simulation was, first of all, an academic research tool. The ”good times” for simulation started with the development of computers. First the analog computers and later the digital computers have boosted simulation to new levels. So, the simulation is now a powerful tool supporting the design, planning, analysis, and decisions in different areas of research and development. Simulation has become a strategic tool in many fields, used by many researchers, developers and by many manufacturers. Of course, robotics as a modern technological branch is no exception. Actually, simulation plays a very important role in robotics, perhaps more important than in many other fields.

Simulation allows us to study the structure, characteristics and the function of a robot system at different levels of details each posing different requirements for the simulation tools. As the complexity of the system under investigation increases the role of the simulation becomes more and more important.

Advanced robotic systems are quite complex systems. Hence, the simulation tools can certainly enhance the design, development, and even the operation of robotic systems. Augmenting the simulation with visualization tools and interfaces, one can simulate the operation of the robotic systems in a very realistic way. Depending on the particular application different structural attributes and functional parameters have to be modelled. Therefore, a variety of simulation tools has been developed for the robotic systems which are used in mechanical design of robotic manipulators, design of control systems, off-line programming systems, to design and test the robot cells, etc.

The simulation tools for robotic systems can be divided into two major groups: tools based on general simulation systems and special tools for robot systems. Tools based on general simulation systems are usually special modules, libraries or user interfaces which simplify the building of robot systems and environments within these general simulation systems. Special simulation tools for robots cover one or more tasks in robotics like off-line programming, design of robot work cells, kinematic and dynamic analysis, mechanical design. They can be specialized for special types of robots like mobile robots, underwater robots, parallel mechanisms, or they are assigned to predefined robot family.

We have presented that the simulation is widely used in all fields of robotics from kinematics and dynamics to industrial applications. Actually, advanced robot systems require sophisticated simulation tools which can model accurately enough the physical world at sufficient speed and allow user interaction. New challenges in the simulation of robotic systems are multi-body dynamics that computes robot and object motions under the influence of external forces, fast collision detection and contact determination, realistic visualization of the robot and environment, and haptic interaction. Advanced simulation tools are the foundation for the design of sophisticated robot systems, for the application of robots in complex environments and for the development of new control strategies and algorithms. The simulation being once a tool for the analysis of a robot system and task planning has become an open platform for developing new robot systems. Not only that the modern simulation tools can simulate and visualize the real world in a very realistic way, they allow to go beyond the reality. Namely, the researchers may build experimental environments according to their own imagination, using robots and technologies which are not available yet. In the end, I believe simulation in robotics has reached a very important role and by using different simulation software, the current and future capabilities of complex robotic systems can be significantly improved.

SIMULATION OF SYSTEMS WITH DYNAMICALLY VARYING MODEL STRUCTURE

Peter Schwarz

Fraunhofer Institute for Integrated Circuits IIS , Design Automation Division EAS
Zeunerstrasse 38, D-01069 Dresden, Germany
Phone: +49 351 4640-730, Fax: +49 351 4640-703
email: schwarz@eas.iis.fhg.de

Many technical systems to be simulated change their properties during simulation. Varying of model parameters or numerical values in equations is the normal situation in simulating nonlinear dynamical systems. Hybrid systems are dynamical systems with interacting continuous-time dynamics (modeled by differential equations) and discrete-event dynamics (modeled by automata or state charts). They arise in many fields, including robotics, embedded systems, transportation systems, process control, biological and chemical systems, integrated circuits, etc. In such hybrid systems some complicated changes may occur:

- the user prepared the exchange of some models by other ones (more simple or more complicated) depending on simulation time or on discrete events,
- discrete events may be the reason for changing the structure of the whole system automatically, e.g. with controlled switches.

Simple numerical model variations are accepted by all simulators but the more fundamental exchange of the model structure leads to complicated mathematical problems. It has to be guaranteed that after a discrete event the correct differential equations are chosen and a set of consistent initial values of the state variables need to be calculated. If the number of state variables is varying than the calculation of the initial values for the next simulation interval is much more complicated as in the case of model variations with a constant number of state variables. Therefore, this problem is mostly solved by the use of “dummy” variables which are unnecessary in some simulation intervals but simplify the numerical solution of differential equations. Investigation of hybrid systems has a history over some decades [1] - [6]. Their simulation is supported by some simulators [7], e.g., Matlab/Simulink, Dymola (http://www.dynasim.se/) and AnyLogic (http://www.xjtek.com/anylogic/), but not all of them support a dynamically varying model structure, e.g., adding and removing differential equations. In some technical areas standards exist for the description of hybrid systems, e.g., VHDL-AMS (http://www.eda.org/vhdl-ams/) and Modelica (http://www.modelica.org/).

An object-oriented approach to handle systems with dynamically varying model structures is presented. The conditions for exchanging models are “observed” by a user-defined monitor block which is an additional element in the system model. The monitor calculates control signals which influence the model structure or the exchange of complete models. The user has to deliver the rules for the calculation of new initial values if their automatic determination is not possible. Also these rules are activated by the monitor. Some of these concepts will be implemented in a new system simulator Mosilab [8] which uses Modelica as input language and is comparable, e.g., to Simulink and Dymola.

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MODELING ENERGY DEPENDENT NUCLEAR REACTION PROBABILITIES FROM POINTWISE MEASUREMENTS INCLUDING FULL COVARIANCE INFORMATION

S: Tagesen; University of Vienna, Austria

Corresponding Author: S. Tagesen,
Institute for Isotope Research and Nuclear Physics
Waehringerstrasse 17, 1090 Wien, Austria
Phone: +43 1 4277-51755, Fax: + 43 1 4277- 51752
email: siegfried.tagesen@univie.ac.at

Abstract. For the design of large and highly complex facilities – like, e.g., the international project ITER [1] – reliable basic data with well established covariance information (uncertainties, correlations) are indispensable. The OECD supports the JEFF project, maintained by the NEA Data Bank, Paris [2], directed to provide those data.

What we have is a pile of – more or less complete – documented measurements, collected from all over the world during the last 50 years. What we need is a set of contiguous tables with reaction probabilities (called "cross sections") as a function of incident particle energy along with reliable covariance information.

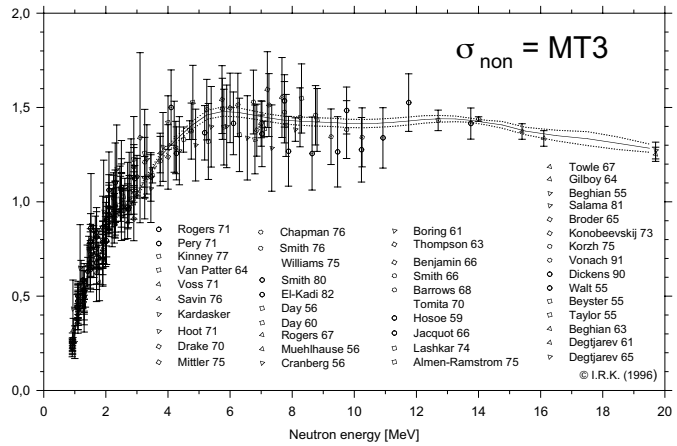

Fig. 1a experimental data and evaluation result

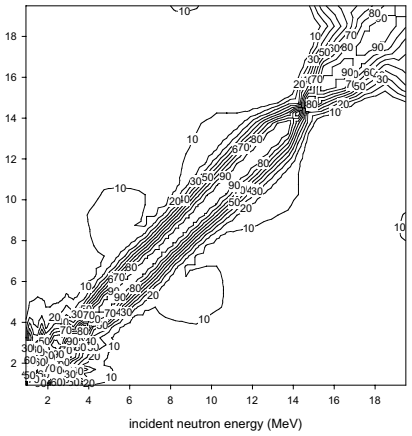

Fig. 1b resulting covariance matrix

Procedures to attain the requirements by means of a Bayesian generalized least squares method and recent approaches using theoretical nuclear reaction codes in combination with Monte Carlo techniques will be discussed and results compared. Particular emphasis is given to the procedures of constructing covariance matrices for the experimental data sets as this determines the quality of the result. Quality assurance procedures within the JEFF project will be mentioned.

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Proceedings
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Modelling and Simulation in Systems Biology

TIME CONSTANTS OF METABOLIC CARBON LABELING SYSTEMS

K. Nöh, S. Adam, M. Weitzel and W. Wiechert, University of Siegen, Germany

Corresponding Author: W. Wiechert
Department of Simulation, Faculty 11/12, University of Siegen
Paul-Bonatz Str. 9-11, 57068 Siegen, Germany
Phone: + 49 0 271 740 - 4727, Fax: + 49 0 271 740 - 3396
email: wiechert@simtec.mb.uni-siegen.de

Metabolic Flux Analysis (MFA) based on ^{13}C labeling experiments (CLEs) aims at the detailed quantification of intracellular fluxes in the central metabolism of a microorganism *in vivo*. Stationary ^{13}C MFA has been established since the 90's as a standard diagnostic tool for the analysis of metabolic networks in the framework of Metabolic Engineering [1]. The backbone of this method is given by the material balances derived under metabolical and isotopical stationary conditions.

One strong limitation of the current stationary method is the requirement of an – at least approximate – isotopic stationary labeling state at the sampling times. This requirement induces a principle lower limit to the duration of a CLE. Motivated by recent experimental and analytical possibilities the refinement of the classical method toward isotopically instationary MFA comes into the focus of interest [2]. The new methodological development is based on repeated sampling during the instationary transient behavior of the ^{13}C labeling dynamics which can be analyzed by highly accurate mass spectrometry methods.

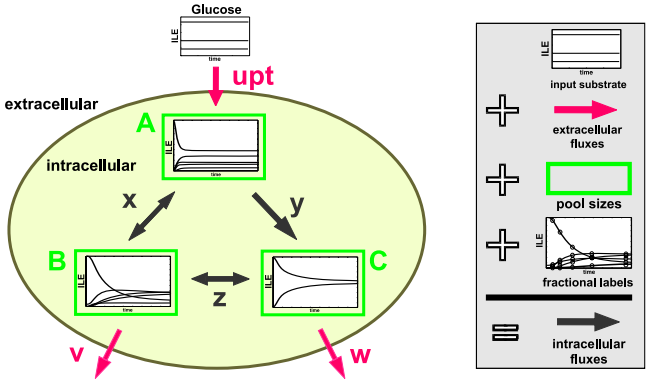

Fig. 1: Principle of instationary ^{13}C Metabolic Flux Analysis.

An instationary CLE can be modeled by a high-dimensional nonlinear differential equation system which exhibits the special structure of a cascade of linear subsystems connected by nonlinear couplings [3]

$$\mathrm{diag}\left({}^{i}\mathbf{X}\right)\cdot {}^{i}\dot{\mathbf{x}} \;=\; {}^{i}\mathbf{A}(\mathbf{v})\;\cdot\; {}^{i}\mathbf{x} \;+\; {}^{i}\mathbf{b}(\mathbf{v}, \mathbf{x}^{\mathrm{inp}}; {}^{0}\mathbf{x}, {}^{1}\mathbf{x}, \ldots, {}^{i-1}\mathbf{x}), \quad i = 1, \ldots, m \tag{1}$$

with ${}^{0}\mathbf{x} = \mathbf{1}$. Because the systems matrices ${}^{i}\mathbf{A}$ are known to be stable, time constants for the labeling enrichment can be defined by their (reciprocal) eigenvalues. By decomposing the linear subsystems into their strongly connected components the complexity of each differential equation subsystem in (1) is reduced in such a way, that it can be solved analytically in a sequential procedure. Thus, all time constants – not only these of the system matrices – can be calculated analytically. Once having determined the time constants they can be related to the unknown parameters of the model given by metabolic fluxes and intracellular pool sizes. This is achieved by computation of the eigenvalue sensitivities. The analytical solution helps to understand the general dynamics of carbon labeling systems in the way the different sub-processes of the labeling dynamics interact.

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CHEMICAL REACTION NETWORK THEORY – A TOOL FOR SYSTEMS BIOLOGY

C. Conradi,[1] J. Saez-Rodriguez, [2] E.-D. Gilles[2] and J. Raisch [1],[2]
Corresponding Author: C. Conradi
[1] Otto-von-Guericke-University Magdeburg
Universitätsplatz 2, 39016 Magdeburg
[2] Max-Planck-Institute Dynamics of Complex Technical Systems
Sandtorstr. 1, 39106 Magdeburg
Phone: + 49 391 67 12732, Fax: +49 391 67 11191
email: conradi@mpi-magdeburg.mpg.de

Systems biology is often concerned with the analysis of large and complex reaction networks, where parameter uncertainty is predominant. Often, however, qualitative knowledge about the dynamics of the system exists, e.g. it might be known from experimental observations that the system exhibits bistability or some other form of multistationarity.
Suppose there are different hypotheses, each corresponding to a different reaction network with uncertain parameters, related to a specific biological process. Suppose furthermore, that a certain qualitative behavior has been observed in experiments. It is then natural to ask which of the postulated networks can, for some conceivable parameter vector, exhibit the observed behavior. We explored this setup in [1].
Recent results from [1] and [2] show that mathematical models of multilayered protein kinase cascades can exhibit multistationarity even on a single cascade level. Using Feinberg's Chemical Reaction Network Theory (CRNT, see e.g. [3]), we showed in [1] that the assumption of a distributive mechanism for double phosphorylation and dephosphorylation is crucial for bistability on the single cascade level, as no model incorporating a processive mechanism for phosphorylation and/or dephosphorylation can admit multiple steady states.
However, in [1], only closed systems were investigated, i.e. the total concentration of the enzymes catalyzing phosphorylation/dephosphorylation, as well as the total concentration of MAPK was assumed to be constant. Using the same approach as in [1], it is possible to show that any one of these assumptions can be dropped, without affecting the result, i.e. multistationarity is still only possible for the network incorporating a distributive kinetic mechanism for phosphorylation and dephosphorylation.
We examine several reaction networks representing a single layer of a protein kinase cascade, each incorporating different mechanisms for phosphorylation/dephosphorylation. The corresponding equations are examined on a mechanistic level, which facilitates the application of Chemical Reaction Network Theory. The advantage of this theory is its independence from particular parameter values. Our results are therefore consequences of the biological hypotheses incorporated in the reaction network, i.e. the particular choice of phosphorylation/dephosphorylation mechanism and not of a particular set of parameter values combined with 'simulations' or 'calculations'.
We consider two possible mechanisms, one distributive and one processive, and three scenarios: (a) a distributive mechanism both for phosphorylation and dephosphorylation, (b) a distributive mechanism for phosphorylation combined with a processive mechanism for dephosphorylation (which is mathematically equivalent to a processive mechanism for phosphorylation combined with a distributive mechanism for dephosphorylation), as well as (c) a processive mechanism for both phosphorylation and dephosphorylation. We investigate (a), (b) and (c), incorporating either conservation of total concentration of MAPK and the catalyzing enzymes or lack thereof for one of either MAPK or the enzymes. We prove that only networks incorporating scenario (a) can show multistationarity. Networks incorporating (b) or (c) cannot admit multiple steady states, no matter what (positive) parameter values are assumed.

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Linear-logarithmic kinetics; a framework for modeling kinetics of metabolic reaction networks

I.E.Nikerel, W.A. van Winden, W.M. van Gulik, J.J. Heijnen, TU Delft, The Netherlands

Corresponding Author: I.E. Nikerel
Technical University of Delft
Julianalaan 67, 2628 BC, Delft, the Netherlands
Phone: + 31 15 278 2352, Fax: + 31 15 278 2355
email: i.e.nikerel@tnw.tudelft.nl

To obtain a better understanding of the behavior of the living cells, it is becoming increasingly relevant to use mathematical models that describe the complex kinetic behavior of metabolic reaction networks that feature metabolite-enzyme interactions (allosteric feedback or feed forward), intercompartmental transport, and cofactor coupling. Although the kinetics of many important enzymes occurring in metabolic networks have been studied extensively for isolated enzymes (*in vitro*), the applicability of these results to describe metabolism of the living cells (*in vivo* metabolism) is doubtful. For example, Teusink et al. showed the discrepancy between the measured *in vivo* concentrations of glycolytic metabolites and the predictions of those using models with *in vitro* determined parameters [1]. This basic problem invalidates detailed models of metabolism based on *in vitro* enzyme kinetics. Therefore, it is mandatory to base the kinetic analysis of metabolic networks on studies on intact cellular networks. These *in vivo* studies use steady state and/or dynamic perturbations to estimate the kinetic parameters of any suitable modeling framework. Such a modeling framework can be a collection of the published mechanistic equations for each of the enzymes in the network, thus basing the presence or absence of specific metabolite-enzyme interactions (but not their strength, i.e. the exact parameter values) on *in vitro* experimental data [2].

Alternative to the classical enzyme mechanistic kinetics, multiple approximative kinetic formats have been proposed in literature (for a review see [3]). The main advantages of the latter are that they have a limited number of parameters and uniform format, which makes them mathematically more tractable, whilst still giving a reasonable description of *in vivo* conditions. Generally, the preferred properties of such models are:

- There is downward concave behavior of rate versus reaction substrate concentration to yield saturation behavior,
- The number of kinetic parameters should be as small as possible,
- Analytical solutions of steady-state network balances are desirable.

Among the approximative kinetic formats suggested in the literature, linear logarithmic (linlog) kinetics has been proposed for modeling of *in vivo* kinetics and for metabolic redesign, and shown to have a good approximation quality, standardized format and relatively few parameters [4]. The parameters in linlog kinetics are the scaled local sensitivities of reaction rates towards metabolite concentrations which happen to be identical to the elasticities as these are defined within the framework of Metabolic Control Analysis.

This paper will focus on several problems which can be fruitfully addressed using linlog approximation. The proposed methodologies will be illustrated with examples.

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DYNAMIC ANALYSIS AND CONTROL OF BIOCHEMICAL REACTION NETWORKS

I. Otero-Muras[1], G. Szederkényi[2], K.M Hangos[2] and A. A. Alonso[1]

[1]Process Engineering Group, Spanish Council for Scientific Research, IIM-CSIC, Spain
C/Eduardo Cabello, 6, 36208, Vigo-Spain
Phone: +34 986231939 Ext 251, Fax: +34 986 292 762
email: antonio@iim.csic.es

[2] Process Control Research Group, Computer and Automation Research Institute,
Hungarian Academy of Sciences
H-1518 Budapest, P.O. Box 63, Hungary

Abstract

Complex dynamics of biochemical networks in the form of steady-state multiplicities or sustained oscillations is a recurring theme in the literature due to its decisive role in physiology of living organisms [6]. Despite they considerable progress concerning network dynamics, the origin of these nonlinear phenomena is still not always well understood and it can not be systematically predicted beyond a case by case basis. This hampers some biological processes being manipulated or monitored at the cell level.

In the present work, we combine concepts and tools from Irreversible Thermodynamics and Control Theory in a contribution to unravel the origin of complexity in biochemical networks. Regarding cells as thermodynamic systems, that are selectively isolated from their environment by means of cellular membranes [4], we can consider their dynamic evolution occuring in terms of the combined action of an endogenous entropy production and the entropy flux associated to the intercell signalling system, in this case consisting of specialized chemicals passing through the membrane. The entropy flux can be meaningfully modified by efficient nonlinear control schemes capable of network stabilization of either steady states or limit cycles [2], and irreversible thermodynamics provide us with the physical insight to further interpret the controlled response.

Based in both the work of Feinberg summarized in [6] relative to the chemical counterpart of biochemical networks, [1] concerning Passivity framework, some underlying structural properties of a general class of networks are studied. Passivity, a concept originated from electric circuitry, may facilitate also the subsequent extension of our results to higher level structures of interconnected systems and signals, such as populations of coupled oscillators [5].

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Visualizing regulatory interdependencies and parameter sensitivities in biochemical network models

S. Noack[1], A. Wahl[1], M. Haunschild[2], E. Qeli[3], B. Freisleben[3], W. Wiechert[2]
[1]Inst. of Biotechn. 2, Research Centre Jülich, Germany
{s.noack, a.wahl}@fz-juelich.de
[2]Inst. of Syst. Eng., Dept. of Simulation, University of Siegen, Germany
{haunschild, wiechert}@simtec.mb.uni-siegen.de
[3]Dept. of Math. and Computer Science, University of Marburg, Germany
{ermir, freisleb}@informatik.uni-marburg.de

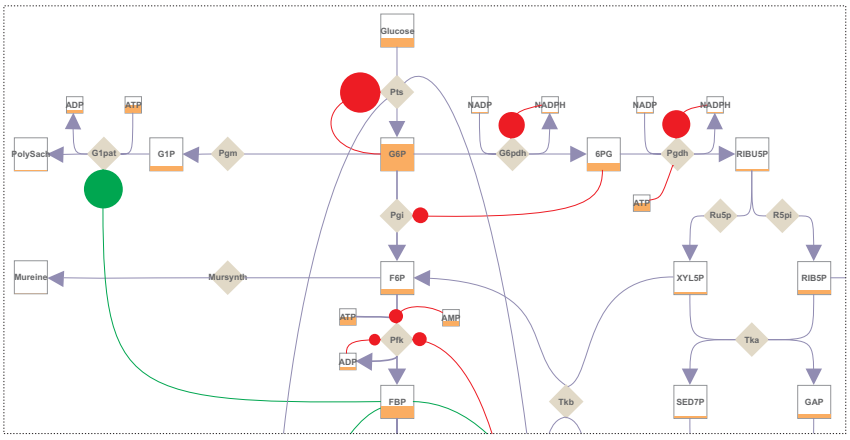
The evaluation of data from Stimulus-Response-Experiments is based on a modeling process. The observed system behaviour is described by a dynamic metabolic model with mechanistic reaction kinetics. With an increase of reaction steps and regulatory interdependencies, e.g. activation and inhibition through modifiers, the amount of simulation data becomes hard to handle.

Here we present the application and extension of methods, which combine visualization and animation of dynamic models to facilitate the analysis of the complex system behaviour. The dynamic changes of metabolite pools and fluxes are simultaneously visualized within the network structure. Depending on the scaling used, different focuses can be set, e.g. observing local dynamics or global concentration balances.

For the visualization of the present inhibition and activation state of certain reaction steps of a metabolic network model a novel quantification method has been developed. The basic idea is to represent the present reaction rate on a scale between the minimal and maximal modifier influence. We set up equations that also allow the quantification of modifier influences in enzyme kinetics with many activators and inhibitors.

Sensitivity analysis of dynamic metabolic network models leads to high-dimensional sensitivity matrices that vary over time. To process the enormous amount of data several visualization techniques are proposed in the literature. We use a colour scale transformation and the reorderable matrix method for the visual exploration of the time-varying matrices.

By this means it is possible to identify patterns or structures locally for a single point of time, e.g., which metabolites or fluxes are strongly influenced through parameter changes. Moreover, global patterns can be found, for example parameters with negligible influence on all metabolite pools and fluxes during the whole course of the simulation. The benefits of our methods are illustrated by a metabolic network model for the central carbon metabolism of *Escherichia coli*.



A HYBRID OPTIMISATION METHOD FOR PARAMETER ESTIMATION IN SYSTEMS BIOLOGY

E. Balsa-Canto[1*], M. Peifer[2,3], J. Timmer[2,3], J.R. Banga[1], C. Fleck[2,3]

[1]Process Engineering Group, Spanish Council for Scientific Research, IIM-CSIC, Spain.

[2]Institute of Physics, University of Freiburg, Germany.

[3]Freiburg Centre for Data Analysis and Modelling, Germany.

*Corresponding author: E. Balsa-Canto, email:ebalsa@iim.csic.es

Most proposed models for cell signalling and metabolic pathways consists of sets of non-linear ordinary differential equations depending on several parameters and initial conditions which might not be amenable to direct experimental determination. Therefore, they must be estimated by fitting the model to experimental data, i.e. by solving the parameter estimation problem.

Parameter estimation is mathematically formulated as a non-linear optimisation problem which often results to be multi-modal. Thus, the solutions achieved by local optimisation methods will highly depend on the initial guess, leading to convergence failures or to local solutions if started far away from the global optimum. This is particularly important in the case of parameter estimation for biological systems, since in most cases no clear intuition even about their order of magnitude exists. Therefore, the development of robust and efficient global methods for properly solving these problems is of the highest interest.

Several strategies have been proposed in the literature which intend to locate global solutions for model calibration. Recently, Rodriguez-Fernandez et al. [2] have suggested an alternative approach which combines a global stochastic with a local deterministic (single shooting) method to take advantage of their complementary strengths: global properties, in the case of the stochastic strategy, and fast local convergence in the case of the deterministic approach. However, in that work devising a robust yet efficient switching point between the stochastic and deterministic method can only achieved after careful investigations and expensive empirical tests.

This work proposes a new hybrid method based on the combination of an evolutionary search approach SRES [3], considered in [2], with a multiple-shooting approach [1]. For the multiple shooting method we employ the generalised-quasi-Newton algorithm equipped with a damping strategy that converges to a full-step procedure in the vicinity of the minimum. This allows us to determine a systematic switching criterion for the transition from the global to the local method.

The applicability and advantages of the proposed procedure for model calibration were analysed through a case study related to the JAK2-STAT5 cell signalling pathway [4]. The results show that the new hybrid strategy presents two advantages over previous alternatives: First, it is equipped with a switching strategy which allows the systematic determination of the transition from the local to global search. This avoids computationally expensive tests in advance. Second, the multiple shooting reduces the multi-modality of the non-linear optimisation problem if compared with the initial value approach (single shooting), therefore avoiding possible spurious solutions in the vicinity of the global optimum.

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CONTROL OF TRAVELLING WAVES IN REACTION-DIFFUSION BIOLOGICAL SYSTEMS

C. Vilas, M.R. García, J.R. Banga and A.A. Alonso*

*Corresponding author: A.A. Alonso
Process Engineering Group, Spanish Council for Scientific Research, IIM-CSIC, Spain.
C/Eduardo Cabello, 6, 36208, Vigo-Spain
Phone: +34 986231939 Ext 251, Fax: +34 986 292 762
email: antonio@iim.csic.es

Reaction-diffusion (RD) mechanisms are central in modelling a number of biological systems such as those describing cell growth and distribution as well as cell communication. One of such models is the so-called FitzHugh-Nagumo (FHN) (see [5]). Slight variations of this model can be used to reproduce the qualitative features of physiological processes such as neural communication or visual perception of the retina. It has been also employed to represent travelling waves that induce the heartbeat or the formation of spirals and irregular fronts, responsible of arrhythmia or fibrillation phenomena of the heart. Dynamic analysis and control of RD systems, and in particular the FHN system, have been the subject of intensive research, especially in what refers to bifurcation analysis leading to moving fronts, spiral waves and pattern formation and their stabilization. In this regard, simple though efficient feed-back control schemes have been recently proposed to unpin or to command the evolution of meandering spiral waves (see for instance [6]).

On the other hand, theoretical work in the control of non-linear RD systems has been mostly focused on the stabilization of given stationary patterns by techniques which made use of the dissipative nature of this class of systems and results in non-linear control theory ([2],[3]). This approach was extended in [1] to develop robust controllers which were able to stabilize arbitrary modes in RD systems.

A typical solution of the FHN system is a plane front which moves throughout the domain without changing its shape. Such a solution is related with the normal behavior of biological systems [4]. Under certain circumstances this front can break giving rise to spirals responsible of biological disorders such as arrhythmia or fibrillation ([4],[5]). Our control objective is to force a system exhibiting the spiral behavior to evolve as a plane front. To that purpose, we take advantage of the dissipative nature of RD systems and make use of results on model reduction of partial differential equations and non-linear control of finite dimensional systems to construct a class of robust feed-back non-linear controllers which ensure limit cycle stabilization. On a spatially distributed domain, this translates into front stabilization. In this way, we make use of a finite dimensional approximation of FHN system and show that such a representation is in fact a good approximation of the original infinite dimensional system. On that basis, a non-linear controller is built and its stabilizing and robustness properties are demonstrated both at a theoretical level and through numerical simulations. Remark that although we concentrate on a particular example of RD system, namely the FHN system, this controller can be applied to other class of RD systems.

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Structural Control

APPROXIMATION OF SHAPE FUNCTIONS WITH A FINITE NUMBER OF ACTUATORS USING TOOLS FROM DIFFERENTIAL GEOMETRY

T. Rittenschober and M. Gusenbauer
Profactor Production Research, Steyr/Gleink, Austria

Corresponding Author: T. Rittenschober
Smart and Adaptive Structures Group
Profactor Production Research
Im Stadtgut A2, 4407 Steyr/Gleink, Austria
Phone: +43 7252 885 - 307, Fax: +43 7252 885 - 101
email: thomas.rittenschober@profactor.at

Abstract. This contribution is concerned with approximating a continuously distributed actuation with a finite number of smart material actuators. This task typically arises in compensating deflections of mechanical structures due to external loadings. In practical applications, however, the mechanical structure is only equipped with a finite number of actuators. Since perfect compensation is unattainable under these circumstances, the actuation voltages have to be chosen such that a measure of deviation from perfect compensation is minimized. Differential geometry allows us to identify conditions under which the deviation of the difference of the Lagrangian densities of external loadings and approximated actuation from being a null Lagrangian is minimized. The derivation of the conditions requires a deeper understanding of the variational derivative, the exterior horizontal derivative, the homotopy operator and their respective interrelations. The entire procedure of determining the conditions is accompanied by an illustrative example given by a simply supported beam equipped with a finite number of equally sized piezoelectric patches under a constant transverse loading, see figure 1.

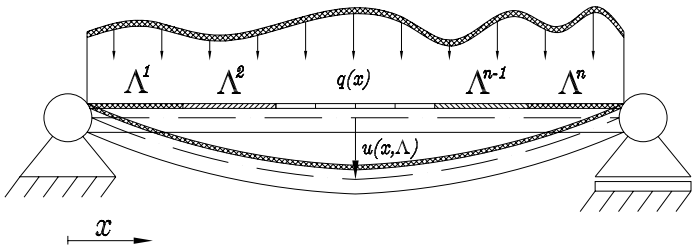

Figure 1: Simply supported beam with n equally sized piezoelectric patches under an arbitrary transversal loading $q\,(x)$.

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DISPLACEMENT CONTROL OF VISCO-ELASTIC STRUCTURES

H. Irschik and M. Krommer, Johannes Kepler University Linz, Austria

Corresponding Author: H. Irschik
Johannes Kepler University of Linz
Altenbergerstr. 69, 4040 Linz, Austria
Phone: + 43 732 2468 9761, Fax: + 43 732 2468 9763
email: irschik@mechatronik.uni-linz.ac.at

The present paper is concerned with the dynamics of a smart structure under the action of transient imposed forces, i.e. of forces that are applied externally. It is assumed that the structure consists of visco-elastic members with actuating elements, and that the latter additional actuation is produced by imposed eigenstrains, e.g. by the electric field acting in piezoelectric layers or stacks that are integrated within the structural members. The actuating elements provide additional actuation forces, which however are internal forces.

As a common formulation in structural dynamics, the smart structure under consideration is modeled by a set of linear ordinary differential equations in time with constant coefficients. For the sake of brevity, we consider homogeneous initial conditions. We assume that the mass, stiffness and damping matrices of the structure are given, as well as the time-evolution of the imposed forces.

Under the action of the imposed forces alone, transient displacements of the structure would take place. Now, the problem addressed and solved in the present paper is the following. We ask for an additional distribution of actuation forces (produced in the structural members by means of eigenstrains that are imposed to their integrated actuating elements), such that the displacements of the structure follow exactly some prescribed trajectories, notwithstanding the fact that imposed forces are present. This problem is denoted as displacement-tracking problem in the following. The latter problem is inverse to the usual direct problem of structural dynamics, namely to compute displacements due to some imposed actions. While this direct problem is known to have a unique solution, at least in the present framework of a linear formulation, the solution of the displacement-tracking problem in general is not unique. Indeed, it will turn out that infinitely many distributions of actuation forces can be imposed to a redundant structure in order to reach the goal of displacement-tracking.

The present paper is devoted to a solution of the displacement-tracking problem by means of a problem-oriented combination of two techniques. One of these techniques is to apply actuation forces such that the goal of zero-displacement-tracking is reached, i.e. that the displacements due to the imposed forces are completely suppressed by the actuation forces. The structure then remains in its undistorted shape despite the presence of the imposed forces. One therefore also talks about shape-control, see Irschik [1] for a review. For shape-control solutions in the framework of the linear field theory of elasto-dynamics with eigenstrains, see Irschik and Pichler [2] and Krommer and Varadan [3]. In the present framework of structural dynamics it can be shown that every self-equilibrating set of actuation forces can be added to a solution of the shape-control problem, which reveals the above mentioned non-uniqueness. Non-vanishing self-equilibrated actuation forces can be produced in redundant (statically indeterminate) structures only. In the latter case, however, the non-uniquenes can be used to conveniently re-design the original shape-control solution. The second technique is to apply the actuation forces in a manner that suppresses the restoring forces (the internal forces) throughout the structure. The structure then remains stress-free despite the presence of the imposed forces. We therefore talk about zero-stress-tracking. For a recent discussion on zero-stress tracking, under static conditions, see Nyashin, Lokhov and Ziegler [4].

The present paper is devoted to show that displacement-tracking can be achieved by combining zero-displacement tracking and zero-stress tracking in a problem oriented manner. Particularly, we present a solution in the framework of the linear theory of structural dynamics. A redundant structure with a single degree of freedom is used as accompanying example.

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STABILIZATION OF A FRAME STRUCTURE - CONTROLLER DESIGN, IMPLEMENTATION AND EXPERIMENTS

J. Schröck, K. Zehetleitner
Johannes Kepler University Linz, Austria

Corresponding Author: J. Schröck
Institute of Automatic Control and Control Systems Technology
Altenbergerstraße 69, 4040 Linz, Austria
Phone: +43 732 2468 - 9733, Fax: + 43 732 2468 - 9734

email: johannes.schroeck@jku.at

In this contribution the stabilization of an experimental setup of a vertical frame structure undergoing horizontal excursions is discussed. The structure consists of 3 storeys connected with flexible links. The actuator is an active mass driver (AMD) on the top level storey. As measurements the acceleration of each storey and the position of the mass in the AMD unit are accessible. The links are modelled as Bernoulli-Euler beams. Using the Lagrange formalism and an appropriate Ritz ansatz for the deflections of the beams, a finite dimensional mathematical model of the entire frame structure is derived. Comparisons using the frequency response of the mathematical model with measurements are provided for model validation.
For the controller design two different types of excitations of the frame structure are considered. In the first case only the upper parts of the frame structure is subject to excursions while the basement remains motionless. The second case is concerned with vibrations of the basement which propagate through the entire structure. In case of a high-rise building the first scenario reflects the case where strong winds cause a libration of the building, whereas the second scenario models an earthquake. However, both of these types of vibrations occur in various applications not only in the field of civil engineering. For each case a discrete LQR (linear quadratic regulator) controller is designed. In addition an LQG (linear quadratic Gaussian) observer is used to estimate the system state from the measured accelerations.
As a main result in this contribution it is shown that for control tasks with a similar time scale in structural control a controller implementation on a personal computer using an open source solution is possible and provides good results. Here, *Debian Linux* is used as operating system extended with RTAI [4], [1]. RTAI (real time application interface) is a hard real-time extension of the Linux operating system licensed under GNU General Public License. The RTAI-Lab [2] graphical user interface (GUI) called *xrtailab* is used to realize the controller and to monitor the system behaviour. The communication with the I/O board is done via an open source driver provided by COMEDI (linux Control and Measurement Device Interface) [3]. Measurements of experimental results with the test stand show the performance of the controller and especially of the overall implementation.

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MATHEMATICAL MODELING, CONTROL AND EXPERIMENTAL VALIDATION OF AN EARTHQUAKE EXCITED ONE-STORY FRAME

D. Huber[1], LCM, H. Irschik[2] and M. Krommer[2], University of Linz, Austria

[1]Corresponding Author: D. Huber
Linz Center of Mechatronics (LCM)
Altenbergerstraße 69, A-4040 Linz, Austria
Phone: +43(0)732/2468/1889, Fax: +43(0)732/2468/9763
email: daniel.huber@jku.at

[2]Institute of Technical Mechanics
Johannes Kepler University of Linz
Altenbergerstraße 69, A-4040 Linz, Austria
irschik@mechatronik.uni-linz.ac.at
krommer@mechatronik.uni-linz.ac.at

The present paper is concerned with the modeling and control of a one-story frame structure, which is excited by an imposed horizontal ground motion of a shaking table it is fixed to. A mathematical model is derived and a controller is designed based on a proper physical model. The dynamics of the structure are modeled using the principle of linear momentum for the rigid floor and the two highly flexible walls are modeled as thin beams taking into account axial forces (second order theory [3]). The equation of motion for the floor is transformed into the Laplace domain, resulting into the transfer function of the structure. As the modeling of the structure assumes the axial force constant and the inertia negligible in the beam equations, the influence of the beam mass on the equation of motion for the floor has to be taken into account. Furthermore, we consider structural damping in the equations. Two parameters are identified using a direct search method algorithm (Nelder-Mead simplex, [2]). Numerical results of the equation of motion are compared to measurements of the laboratory setup and a very good agreement is found. For the control of the structure, piezoelectric patches are applied to the walls and used as both sensors and actuators. The arrangement of the sensors and actuators is collocated, with the sensor measuring an approximation for the relative displacement of the floor. Stiffness and mass of the patches are taken into account by means of the above described parameter identification. As the structure represents a port controlled Hamiltonian system with dissipation with collocated sensors and actuators, see [1], a PD - controller can be used to control the relative displacement of the floor. Experimental results are presented, in which the efficiency of the control strategy for the control of the relative displacement of the floor is validated.
The present contribution is part of the RIO-SCN, which aims at bundling existing expertise in Structural Control in Upper Austria involving partners from Academia (Institute for Technical Mechanics and Institute of Automatic Control and Control Systems Technology at the Johannes Kepler University Linz), Research Centers (Linz Center of Mechatronics and Profactor) as well as Technology Management (Upper Austrian Technology Management and Regional Development Agency) to establish university and industry relationships and to conduct industry projects requiring a multidisciplinary effort. The scientific partners of the project aim to establish applications to demonstrate the effectiveness of active methods for structural control. The present paper points out recent results of this effort.

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COMPENSATION OF FLEXURAL VIBRATIONS IN A CANTILEVER USING DISTRIBUTED PIEZOELECTRIC SENSORS AND ACTUATORS

M. Nader*, H.-G. v. Garssen†, H. Irschik‡

*Corresponding Author: M. Nader
Linz Center of Competence in Mechatronics
Altenbergerstrasse 69, 4040 Linz, Austria
Phone: +43 70 2468-9768, Fax: +43 70 2468-9763
email: manfred.nader@lcm.at

†Siemens AG Munich, CT PS 8
Otto-Hahn-Ring 6, 81729 Munich, Germany
hans-georg.garssen@siemens.com

‡Institute of Technical Mechanics
Johannes Kepler University of Linz
Altenbergerstrasse 69, 4040 Linz, Austria
irschik@mechatronik.uni-linz.ac.at

The compensation of flexural vibrations gains more and more importance, especially in the field of automotive and aircraft applications. In the present contribution the concept of dynamic shape control by the use of piezoelectric actuation is applied to annihilate emerging disturbing vibrations. The goal of shape control is to nullify disturbing structural deformations by means of a distributed control actuation. In practice, this means to prescribe the spatial distribution or the shape of the actuation, together with its time evolution, such that the total displacement field vanishes throughout the entire structure. The basic idea is derived for the case of a simple structure represented by a slender cantilever. The support is moved harmonically, thus flexural vibrations are occurring in addition to the prescribed rigid body motion. The goal is to actuate distributed piezoelectric patches, so that vibrations are nullified within the entire beam at every time instant. In the present contribution a continuous distribution of piezoelectric actuation is determined first. The deflections can be compensated all over the beam at every time instant, if the actuating moment coincides with the negative quasi static (statically admissible) bending moment assuming homogeneous initial conditions. The result of the shape control problem is validated by means of finite element computations. The actuation is discretized to a finite number of piezoelectric patches, see Fig 1.

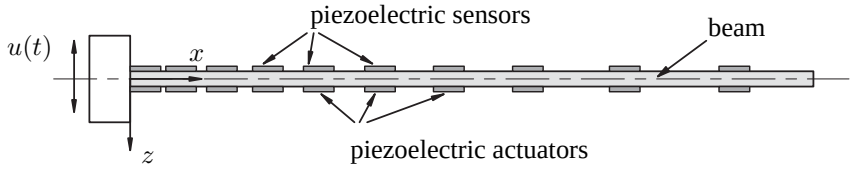

Figure 1: vibration compensation in a beam using distributed piezoelectric patches

The positions and number of piezoelectric actuators is suggested via static and harmonic finite element computations within the program code ANSYS. A laboratory setup is used to validate the analytical and numerical results. The performance of the system is increased by the use of a feedforward control design, assuming the disturbance is known or can be measured in advance. The different sections of the system are realized by using finite impulse response (FIR) filters. A part of the system is identified offline by a least mean square (LMS) algorithm. Based on MATLAB/SIMULINK, an adaptive control algorithm (FX-LMS) is designed and implemented on a dSPACE DS1103 PPC controller board in order to identify the critical part of the system online. Thus, inverting the artificial generated signal by the controller board and applying it to the piezoelectric actuators compensates the occurring flexural vibrations of the system. In the case of an unknown disturbance a feedbackward control design is investigated. Based on frequency response measurements of the smart structure a disturbance controller is designed. According to the introduced theory of dynamic shape control the model of the cantilever is represented by a SISO system reducing the complexity of the control strategy under consideration.

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Modelling Methods and Techniques

DUALITY OF LINEAR SYSTEMS: A BOND GRAPH PERSPECTIVE

Stefan Lichiardopol and Christophe Sueur

L.A.G.I.S., Ecole Centrale de Lille,
Cité Scientifique, BP48
59651 Villeneuve d'Ascq Cedex, France
Phone : +33 3 20 33 54 14
e-mail: stefan.lichiardopol@ec-lille.fr, sueur@ec-lille.fr

The main concept which is discussed throughout this paper is the duality. Duality may seem as a rather philosophical concept, but system modelling and control have a few aspects in which the duality can be clearly seen. Everyone knows about duality between controllability and observability. Extended research has been carried out on this topic especially regarding the LTI systems.

Unfortunately there is a gap when the concept of duality has to be extended to linear systems (time-varying included), or to nonlinear systems in general.

The concept of duality in linear systems has been discussed from the state space representation point of view in [4], [6] in the 80's. In the late 90's, the module theoretical approach introduced by Fliess [3] offered a new perspective [5].

The present paper brings a new perspective by using the bond graph, a graphical tool which can be seen at the same time as a state space representation and as a module. Therefore the procedures developed in both approaches can be applied on the bond graph models. The interest of the article is the application of the duality concept in system analysis. Using the recent results in [1], [2] the scope of the paper is enlarged over the nonlinear models by using the variational bond graphs.

Firstly, the paper offers a recall of the duality from the two approaches, state space and module theoretical representations. Afterwards the aim is on the definition of the dual bond graph model. Then, the procedures used to prove the duality in system analysis from the bond graph perspective are presented. All the developed techniques are applied on an example, with the analysis of a separately excited DC motor. For the application two models are used: a simplified time-varying model and a nonlinear model, by using the variational bond graph.

This paper is a gateway to a new perspective of dealing with the linear systems and opens new perspectives on other duality. Future work involves (A,B)-invariance and (C,A)-invariance, system decoupling and disturbance rejection by state feedback and output injection, as well as possible generalization for the nonlinear case using the variational bond graph model.

On the long range the aim is to provide a comprehensible tool for the engineers which are proficient in either command or observers and who, based on their strong point, can easily build a good system regulation using the duality of the system and the procedures which are most familiar to them.

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AN OPTIMAL CONTROL PROBLEM: BOND GRAPH REPRESENTATION AND SOLVER IMPLEMENTATION

Bogdan Chereji [1] , Omar Mouhib [1] , Wilfrid Marquis-Favre [1]
Daniel Thomasset [1] , Jérôme Pousin [2] , Martine Picq [2]
(1) Laboratoire d'Automatique Industrielle [1]
(2) Institut Camille Jordan [2]
Institut National des sciences Appliquées de Lyon
25 [1] ,21 [2] , avenue Jean Capelle
F-69621 Villeurbanne Cedex
Phone: +33 (0)4 72 43 81 98 Fax: +33 (0)4 72 43 85 35
e-mail: <firstname>.<lastname>@insa-lyon.fr

Abstract. The importance of energy loss minimization in a real industrial environment is substantial, especially nowadays, where every small loss is critical. Also, the multidisciplinary character of the problem addressed makes the use of traditional methods tedious, so the technological level of modeling cannot satisfy the needs. Unfortunately, the mathematical level does not suit either, so the use of a physical level modeling language is advantageous. Bond graph language has proved itself a very efficient tool in modeling, analysis and the design of mechatronic systems, especially by energy and dynamic point of view [2].
The work presented in this paper, although it concerns optimal control, applies this effort at different levels. The framework of this research belongs to a more general task of dimensioning mechatronic systems. The optimal control implementation constitutes one of the phases that has to be overcome, in order to advance in the direction of the virtual prototyping of these systems.
The class of the problem concerns linear time invariant single input single output systems, where the performance index corresponds to dissipative energy. The control variable is taken into account also as dissipative loss, using a weighting factor.
The paper is organized in 4 sections. The first two deal with the bond graph representation of an optimal control problem. In the first section, a systematic procedure aims at automatically generating the bond graph representation of an optimal control problem having the bond graph representation of the system under study as its starting point. The steps are listed, and it should be noted that this procedure only takes place at a graphical level, skipping the symbolic developments usually implied by the use of the Pontryagin methods.
The second section familiarizes the reader with the use of the procedure shown in the first section. A rather simple (a second order linear system) example is used. The model follows the procedure described in the first section, which provides as output the bond graph model corresponding to the specified optimal control problem. The analytical developments are then carried out, just to confirm that the result obtained by the proposed bond graph approach corresponds to the one obtained by applying the classical Pontryagin procedure.
The second part of the paper deals with the numerical issues. First, as the Pontryagin principle leads to a particular case of boundary value problems (TPVBP) [1], a brief study about the suitable techniques for solving them is performed. The first subsection includes the theoretical developments necessary to explain the motivation for the practical method implemented here. This section also contains a small paragraph to expose the research framework, and the basis for choosing the method. This section also reveals the practical means for solving the two point boundary value problem.
A software was created especially to address the problem and used on the same example as the one treated in the second section.
Finally, the conclusions are pooled. The limitations of the procedure and perspectives for future research are then discussed.

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RELATIONSHIPS BETWEEN MODEL INVERSION AND INVERSE SIMULATION TECHNIQUES

Linghai Lu, D.J. Murray-Smith and E.W. McGookin, Glasgow, UK

Corresponding Author: Linghai Lu,
University of Glasgow
Room 108, 72 Oakfield Avenue, Glasgow, G12 8LT, Glasgow, UK
Phone: +44 141 330- 6137
Email: linghai@elec.gla.ac.uk

Much progress has been made both in the field of inverse simulation and in model inversion in the last decade. Mature approaches to model inversion have been developed for minimum-phase and nonminimum-phase systems. However, most are quite tedious and complicated to apply in practical situations especially in the aircraft field. The primary objective of this paper is to explore and highlight the close relationship between these two mature techniques. The similarities and shortcomings, existing in these two methods, are presented. This research aims to use inverse simulation to develop robust tracking controllers based on the traditional output-tracking control system structure, thus avoiding the more complicated techniques of model inversion.

Traditionally, inverse simulation has not been used for output-tracking and inversion-based controllers. This is partly due to the limited computational speed of computers available at the time. In addition, earlier investigations of inverse simulation methods have not considered the applicability of this approach for the special case of nonminimum-phase systems. The results point out that, provided a suitable value of discretized time interval is used, inverse simulation can be applied instead of model inversion for a minimum-phase system. This is illustrated by an application involving a nonlinear HS125 fixed-wing aircraft model. Moreover, it is shown for the first time that inverse simulation also solves the nonminimum-phase problem for linear systems in a natural and more straightforward way compared with the model inversion approach. This development depends upon zero redistribution within the process of inverse simulation and provides a link between the linear inverse system and its discrete counterpart in a mathematical sense. This has been successfully proved with an example of an eighth-order linear Lynx helicopter model.

CONCEPTS FOR HIGH PERFORMANCE GENERIC SCIENTIFIC COMPUTING

R. Heinzl, P. Schwaha, T. Grasser, CDL for TCAD, Institute for Microelectronics, TU Vienna, Austria
M. Spevak, Institute for Microelectronics, TU Vienna, Austria

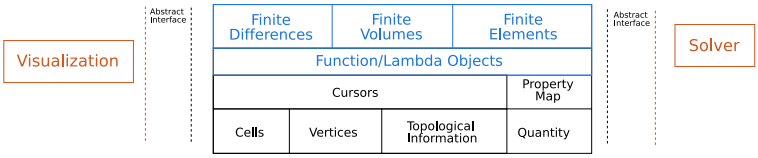
Corresponding author: R. Heinzl
TU Vienna, Gusshausstr. 27-29/E360, A-1040 Vienna, Austria
Phone: +43 1 58801-36053, Fax: +43 1 58801-36099
email: heinzl@iue.tuwien.ac.at

The scientific computing approach is used to gain an understanding of scientific and engineering problems by the analysis of mathematical models implemented in computer programs and solved by numerical techniques. Due to the diversity of the mathematical structures, combined with efficiency considerations, in particular in three dimensions, the development of high performance simulation software is quite challenging.

We have identified the following issues for an environment suitable for scientific computing: sophisticated real-time visualization possibilities, high performance, abstract solver interface, automatic treatment of discretization schemes, and algebraic support for an easy implementation of equations. To deal with all of these issues, our institute has developed different simulation environments, libraries, and applications during the last decade. However, none of these simulators has proven to be perfect for the rapid progress in scientific software development. Even the reuse of simple code parts is difficult, due to the non-generic-library approach.

We compare the following libraries suitable for TCAD or scientific compuing: Blitz++ [1], Matrix Template Library (MTL, [2]), Boost Graph Library (BGL, [3]), CGAL [4], GrAL [5], Prophet [6], and deal.II [7]. We have extracted the main concepts from our own simulation tools and have combined them with the most promising techniques proposed by other groups. The result of this work is the multidimensional and multitopological *generic scientific simulation environment (GSSE)*.

The approach used for the development of GSSE fundamentally relies on the generic programming [8] and functional programming paradigm [9]. Generic programming, started with the development of the STL, is an especially attractive paradigm for the development of libraries for high-performance computing because it emphasizes generality and efficiency simultaneously. With this approach libraries can be coupled much more tightly to compilers, allowing libraries to provide highly-reusable data types and algorithms, as specific optimization possibilities as well. The base concept of GSSE is the separation of topology, in this case discrete topology, and quantities, which means all different kinds of attached properties. The geometrical information, for example coordinates for a vertex, can be seen as some kind of quantity. This case is illustrated in the next figure by the separation of the cursor concept and the property map concept, where the cursor concept uses only topological information. The abstract interface mechanism to the visualization and the solver capabilities are also included in the figure.



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MODELLING AND STABILITY ANALYSIS OF LINEAR SWITCHED SYSTEMS VIA TOPOLOGIC CONSIDERATIONS USING GRAPH THEORY

M. de la Sen and A. Ibeas, UPV/EHU, Spain

Corresponding Author: Asier Ibeas
Department of Systems Engineering and Automatic Control
Faculty of Sciences. University of Basque Country
Aptdo. 644- Bilbao. 48080- Bilbao. SPAIN
e-mail: iebibhea@ehu.es

The stabilization of dynamic systems is a crucial research topic from several decades. Thus, there are in nature time-varying systems defined via switches trough time in-between several configurations which may be time-variant or time-invariant. *A serious inconvenience to analyse those systems by conventional techniques is that their properties depend on the basis chosen to represent the system in state-space* [1], or in other words, on the model of the system. Examples are the use of descriptions consisting of linearized models around different equilibrium points which describe certain chemical processes or the configurations including switches between several estimation algorithms in parallel multiestimation schemes which set more efficiently the identification performances through time than conventional single estimation schemes, [1,3]. Those schemes are sometimes used in tandem configurations with associated adaptive controller parameterisations to improve the tracking performances in adaptive control compared to the use of single adaptive controller parameterisations, [2-5,8].

In this paper, the stability of general configurations consisting of a set of parameterisations with switching in-between them is discussed from topological considerations using standard graph theory and an "ad-hoc" axiomatic framework constructed from a set of previous background of analytical results.

Firstly, the description and modelling of the hybrid switched system is developed using graph theory. Then, some analytic previous results on global stability (GS) and global asymptotic stability (GAS) of hybrid dynamic systems are introduced in order to able to settle the axiomatic framework used to investigate the general topologically-based stability results, [1-4]. Hence, a set of axioms is stated in order to then formulate the main results concerning stability issues. It is well-known the fact that when dealing with very general classes of systems, Expert Systems formulated *ad-hoc* for certain applications in a expert rule-based context of Artificial Intelligence, *the clear formulation of an axiomatic context is crucial to then derive new results which should agree with the empirical observation or knowledge as well as with results obtained from conventional mathematical techniques*, [7]. The axiomatic context is then used to obtain stability results for a general class of hybrid systems, mainly based on the topology of the links between the various configurations associated with a state trajectory as well as on the nature of the vertices related to the stability of the various isolated parameterisations.

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ON NUMERICAL SOLUTION OF ARBITRARY SYMMETRIC LINEAR SYSTEMS BY APPROXIMATE ORTHOGONALIZATION [1]

Constantin Popa, OVIDIUS University of Constanta, Romania
Blvd. Mamaia 124, 900527 Constanta, Romania
Phone: +40 241 618070, Fax: +40 241 618372
email: cpopa@univ-ovidius.ro

In the last 20 years the field of inverse problems has certainly been one of the fastest growing scientific areas. This growth was largely been driven by the needs of applications both in science and industry. But, unfortunately the mathematical modelling techniques for such problems give rise to various kind of equations which are not well-posed in the sense of Hadamard, i.e. to so called *ill-posed problems*. A very important class of inverse problems are those modelled by integral equations of the first kind. We can mention in this sense the Radon inversion in X-ray tomography, time resolved fluorescence in physical chemistry, signal and image processing, heat conduction, the determination of charge distribution generating a given electric field and many others (see for details the well known monographs [1], [3]). We shall consider through this paper first kind integral equations of the following model form: for a given square integrable function y on the real interval $[c, d]$, find a similar one x such that

$$\int_c^d k(s,t)\ x(t)dt \ = \ y(s),\ s \in [c,d], \tag{1}$$

where $k(s,t)$ is the kernel of the equation, which we shall suppose to be continuous. In order to solve the above mathematical model (1) we first need a discretization of it. Among many possibilities in this sense, we considered in the present paper the method of collocation, according to which (see for details [2]), after we fix n collocation points in $[c,d]$, $c \leq s_1 < s_2 \ldots < s_n \leq d$ we associate to (1) the linear symmetric and positive semidefinite system of equations

$$Ax = b,\ (A)_{ij} = \int_c^d k(s_i,t)k(s_j,t)\mathrm{dt},\quad b(i) = y(s_i), i,j = 1,\ldots,n. \tag{2}$$

Then, the approximate solution for (1) is given by $x^{approx}(t) = \sum_{i=1}^n x_{LS,i}\ k(s_i,t)$, where $x_{LS} = (x_{LS,1}, x_{LS,2}, \ldots, x_{LS,n})^t \in I\!R^n$ is the minimal norm solution of (2). Thus, in order to get an enough good approximate solution x^{approx} we need an enough accurate solver for the system (2). In this sense we propose in the present paper a stable and robust iterative algorithm, based on a modified version of the one that we proposed in [4]. We prove convergence of our method for symmetric and positive definite systems like (2). In the last section of the paper we also present some numerical experiments on a mathematical model of an inverse problem concerned with the determination of charge distribution generating a given electric field.

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Shapes and algorithm for determining signals maximising the absolute value of error

Edward Layer and Krzysztof Tomczyk
Cracow University of Technology,
Faculty of Electrical and Computer Engineering,
ul. Warszawska 24, 31-155 Kraków , Poland
pelayer@cyf-kr.edu.pl
petomczy@cyf-kr.edu.pl

In measurement of dynamic signals the value of absolute error is of essential importance, especially for tracking systems and systems intended for measurement of signals shape. Such systems are commonly applied in many different branches, e.g. in electrical metrology (transducers, filters, strain gauge amplifiers, measuring microphones etc.), in geodesy (accelerometers, vibrometers etc.), in medicine (electroencephalographs, cardiographs etc.), in meteorology (autocomparators, autobridges etc.). For systems of such type input signals are unknown and can not be determined in advance. Also the rated operation conditions of these systems are very difficult to define as they usually work in a dynamic mode, far from a steady state. For that reason there is no point in determining the errors by means of typical standard signals as the results received depend essentially on the input signals for which they are computed. Moreover, in practice real systems are not excited by standard signals, but usually by unknown dynamic signals which are decidedly different from the standard ones. It should be noted, however, that the solution of a problem posed in a way which could make the error values independent of the input signal form is possible for maximum errors. But the procedure of determination of maximum errors requires special input signals to be used, which warrant that the error values determined with them will always be higher or at least equal to the value generated by any other signal. Below we will determine shapes of such signals constrained in magnitude, and simultaneously in magnitude and rate of change.

The paper presents a method and algorithm for determining input signals which maximise the dynamic error expressed by means of its absolute value. Being maximum, the values of these errors are valid for any dynamic signal which might occur at the input of a real system. In this way all the possible signals are taken into consideration at the same time. It should be stressed that these can be non-determined signals whose form cannot be predicted a priori. Two types of signals are taken into consideration: signals with a magnitude constraint and signals constrained in magnitude and rate of change. Solutions derived in the paper enable calculation of the absolute value of error by means of analytical formulae which give precise results and can be realised in a very short time.

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MULTISTEP FRACTIONAL-RATIONAL NUMERICAL METHOD FOR STIFF DYNAMIC PROBLEMS

Roksolyana Stolyarchuk
National University "Lvivska Politechnika"
Institute of Applied Mathematics and Fundamental Sciences
Bandera str.,12, 79013 Lviv,Ukraine
Phone: +38 032 2370557, Fax: + 38 0322 630311
email: roksols@yahoo.com

This work presents a new computational approach for the analysis of stiff dynamic systems by construction of semi-explicit fractional-rational numerical methods with modification of integration step.
Mathematical models of real-life dynamic processes are frequently describes by complicated nonlinear stiff systems of ordinary differential equations (ODEs). The numerical approximation of such stiff differential equations continues to be one of the principal concerns of numerical analysis. In the works of Curtis, Hirschfelder and later Dahlquist [2] have been shown that explicit numerical methods for investigation of stiff systems are ineligible and ineffective because they have a bounded region of stability. For implicit Gear's methods Dahlquist's barrier takes place, they don't provide required accuracy on whole integration interval and their realization, requires repeated solution of systems of nonlinear algebraic equations.
The performance of proposed numerical methods is considered on the Cauchy initial-value problem $y' = f(x, y)$, $y(0) = y_0$, where $y \in R^N$, $f : R^{N+1} \to R^N$ on some interval of change of an independent variable $x \in [0, x_k]$.

Explicit numerical methods for ODEs are based on linear polynomial Taylor's approximation of systems solution. We can use fractional-rational approximation in the form

$$y_{n+1}^{[p]} = \frac{T_{p,n} + \sum_{i=1}^{p} (-1)^i a_i h^i J_n^i T_{p-i,n}}{E + \sum_{i=1}^{p} (-1)^i a_i h^i J_n^i},$$

where $y_{n+1}^{[p]}$ - is the pth order approximations of solution in grid node x_{n+1}, $T_{k,n}$ -is the kth order Taylor's approximations of solutions of problem in the grid node x_{n+1} relatively to grid node x_n, α_k - the free parameters, which are used for ensure the type of stability with assumption that system have the unique solution J_n - Jacobean matrix of right parts of system in the grid node x_n.
The structure of fractional-rational approximations allows, by using special linear multistep numerical method with excess information, to construct multistep fractional-rational numerical methods, characteristic equation of which hasn't "parasitic roots".
Fractional-rational method for solving stiff systems was tested on benchmark model. Analysis of reduced results confirmed the efficiency of fractional-rational numerical methods, which provided required accuracy on whole integration interval by decreasing numbers of integration step. This leads to decreasing of computing costs and integration time.
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INVESTIGATION OF STRUCTURE OF DYNAMIC PROCESS MODELS VIA SIMPLIFIED REPRESENTATION GRAPHS

A. Leitold and M. Gerzson, University of Veszprém

Corresponding Author: A. Leitold
University of Veszprém
Egyetem str. 10, 8201 Veszprém P.O.B 158, Hungary
Phone: +36 88 624-227, Fax: + 36 88 624-521
email: leitolda@almos.vein.hu

The structure of process models described by semiexplicit DAE systems can be analyzed via representation graph [1, 2]. In our earlier works we have investigated the relationship between the structure of the representation graph and the computational properties of the model (structural solvability, decomposition, calculation path, differential index, dynamic degree of freedom, etc.) [3, 4]. The graph representation can also be used to investigate the effect of the modification of the variable specification or the model transformations on the computational properties [5].

The models of real systems are large sized, in general and their representation graphs are very complex. At the same time these large models (especially in case of the models of technological systems containing several similar process units or the models of cascade systems) consist of model equations which are very similar to each other consequently, their representation graphs contain several similarly structured subgraphs.

In this recent work our aim is to propose an algorithm for the determination of vertices or subgraphs which have the same role from the viewpoint of calculation path. The simplified representation graph can be get as a result of the application of the lumping transformations on these vertices and subgraphs. The simplified representation graph can be used similarly to the original graph for the determination of several computational properties (structural solvability, differential index, e.g.).

The first step is to define the concept of homogeny input vertices and isomorphic subgraphs on the representation graph from the viewpoint of calculation path.
Two types of lumping transformations have been introduced:

- the lumping of homogeny input vertices,
- the lumping of isomorphic subgraphs which are isomorphicly structured L-components being on the same hierarchy level,

and their application conditions has been determined, too.

Applying of the lumping transformation steps we can get graphs with simpler structure (i.e. they contain less vertices), but these simpler graphs unchangeably reflect the structure of the model and its computational properties.

It has been proved although the possible lumping transformation steps can be done in different ways at a given model, there exists a sequence of the possible lumping transformation steps which gives the simplest representation being equivalent with the original model from the viewpoint of the computational properties.

We illustrate our proposed method on a simple model of the granulator drum.

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COGNITIVE MODELING TO REALIZE AUTONOMOUS BEHAVIOR IN MOBILE ROBOTICS

E. Ahle and D. Söffker, University Duisburg-Essen, Germany

Corresponding Author: E. Ahle,
University Duisburg-Essen
Lotharstr. 1, 47057 Duisburg, Germany
Phone: +49 (0)203 379 3022, Fax: + 49 (0)203 379 3027
email: ahle@uni-duisburg.de

This contribution demonstrates the application of a cognitive modeling technique to realize autonomous behavior in mobile robotics as an example of a cognitive technical system. A special situation-operator-model (SOM) is used to structure the reality and map this structuring to a mental model of the system to enable planning and learning. The presented architecture builds the framework for autonomous behavior, and the mental model of the system is maintained and refined by cognitive functions.

The modeling of the human-machine-interaction gives ideas to transfer the understanding of the knowledge-guided human control and interaction, and to use the developed modeling technique to realize "intelligence of machines" [5]. Core of the cognitive behavior is the structuring of real world changes by the situation-operator-model and the information-oriented formalization of the approach [6] allowing the modeling of structural changes within the environment of humans or "perceiving" machines. A comparison of the cognitive model used in this contribution with known and commonly applied theoretical models is given in [7], outlining the advantages of this modeling technique. In [1], the concept of the proposed architecture is explained in detail and first results are shown. One or more goals are provided to the system and have to be translated into the SOM-description. While the planning module requests information from the knowledge base, the learning module modifies and updates the knowledge base, which represents the learning capability of the autonomous system. Furthermore, the cognitive functions organize the situation interpretation, whose technical realization is novel. The idea of perception interdependence is known in advanced modeling of human cognition [2]. The application of the proposed approach is described for a mobile robot as an example of an autonomous system as well as experiences with this approach in a real world environment. As mobile robot the commercially available Pioneer 3 DX from ActivMedia Robotics is used to test the architecture. This autonomous system interacts within a laboratory environment and performs pick and place tasks of colored objects. The autonomous system details the knowledge itself by updating the transition probabilities and applying heuristics introduced in [3, 4]. Three test runs of the realized architecture in a laboratory environment are shown and the refinement of the knowledge base by the system is explained in detail.

The main contribution is the demonstration of the functionality of the autonomous generation of a mental model. Furthermore, the application of the knowledge-based cognitive system to a robotic system interacting with unknown environments is shown. The proposed approach realizes a new quality of flexible and situated interaction of machines especially due to the implemented learning abilities.

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COGNITIVE APPROACHES REALIZING FLEXIBLE INTERACTION BEHAVIOR OF COGNITIVE TECHNICAL SYSTEMS: A COMPARISON

D. Söffker, University Duisburg-Essen, Germany

Chair of Dynamics and Control
University Duisburg-Essen
Lotharstr. 1, 47057 Duisburg, Germany
Phone: +49 (0)203 379 3429, Fax: + 49 (0)203 379 3027
email: soeffker@uni-duisburg.de

Abstract. The application of feedback mechanism to technical systems is one the most important steps improving the dynamics of technical systems and also to realize new technical solutions. The use of models as a base for control leads to a broad range of successful applied methods. The paper focusses to systems where a) equation-based models are not available or not suitable, b) systems are mainly defined by structural changes, c) system or structural changes can neither be determined nor known. This contribution introduces to the ideas, basic concepts and potentials of cognitive architectures, typically used describing Human-Machine-Interaction or artificial intelligence-oriented approaches realizing flexible interaction of systems/controllers. Known archictectures are briefly introduced and compared within usual criteria PIPE (Perception/Interpretation/Planning/Execution) and new criteria related to their practicability and adaptability to replace technical control approaches introduced and detailed within this contribution.

1. What is cognition?

Following the definition of Strube [1],

- cognition decouples the inputs and the outputs (typically of the considered human behavior),
- allows the anticipation of intented actions as well as the storage of experiences, and
- is neither related only to humans or animals [1] nor to psychology (comment of the author).

Cognitive archictectures / an or approaches developed for Human-Machine-Interaction or modeling Human-Task processing implicitly or explicitly claim to deal with more complex systems. The idea to apply cognitive-based control approaches to give technical systems more adaptivity and flexibility is given in [15].

2. Known Architectures

All approaches to be compared are so-called macro-cognition [2] approaches, so claim to model the cognitive behavior on a phenomenological level [3].

3. Criteria for Comparison of Cognitive Archictectures with the Aim of Technical Realization related to Technical Systems

The criteria to compare the approaches are strictly related to theoretical aspects with respect to the internal organisation of the approaches and to practical aspects related to the realizability with technical systems with respect to realize cognitive technical systems.

4. Comparison

The contribution extends the review given in [2] by considering new approaches and especially by detailling and adding aspects necessary for realization, which are usually neglected for HMI-oriented approaches usually given on a describtive level . The comparison outlines the development within this new ideas and details different aspects of the internal structure of the mostly information-science oriented approaches. It is shown that the structural concept of the internal structure is important for realizing cognitive technical systems. The ability of the approach to integrate the ‘world’ model into the memory and the relation to cognitive functions PIPE in combination with principal realizability for programming seems to be the key feature with the approaches to realize cognitive technical systems as ‘intelligent’ machines.

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A USER-INTERFACE FOR EXPLORING LARGE GRAPHS

Stefan Wiegreffe, Universität Hamburg, Germany

Vogt-Kölln-Str. 30, 22527 Hamburg, Germany
Phone: + 49 40 42833-2437, Fax: + 49 40 42833-2552
email: wiegreffe@informatik.uni-hamburg.de

While graph-based structures are increasingly common these days in such different application areas as content management (RDF, ontologies), system performance simulation (Petri Nets) and psychology (cognitive maps), everyday systems that actually implement such techniques are far from widespread. Part of the problem is a lack of applications with well designed user-interfaces to support the graph-paradigm.
Interfaces for graph-based structures can usually be split up into two groups: The first group being interfaces that calculate and render a visualization of the underlying graph structure. They in general have a problem with large graphs. On the one hand, the bigger the graphs get, the more screen real estate they need. Very soon, it becomes impossible to draw a full graph on a screen. On the other hand, the calculation of a good representation of the graph (i.e. a representation that sticks to certain formal aesthetic criteria), is usually NP-hard, making it impossible to calculate a proper visualization of the graph in a reasonable amount of time.
The second group of interfaces totally omits a visualization of any kind. This avoids the mentioned problems, but on the users side, this leads to a lack of orientation, commonly known as *Lost-in-Hyperspace-Problem*. The usual means against this problem are visualizations of the content-structure. Besides the problem of disorientation, recent research results show that hyperspaces without proper visualization are nearly useless to people who hadn't created them.
So obviously we need some kind of mixture of these two types of interfaces, eliminating the drawbacks while keeping the advantages of the respective interface type. Basically, the idea is to show all neighbors of an already drawn node. The neighbors are not displayed in full detail, but their presence is clearly shown. Users can then expand the neighbor-nodes interactively. The expanded nodes will then be shown in full detail and with their respective neighbors. This way, users can build their own visualization of the graph on a step-by-step basis. The drawbacks of this concept have to be neutralized within a proper user-interface.

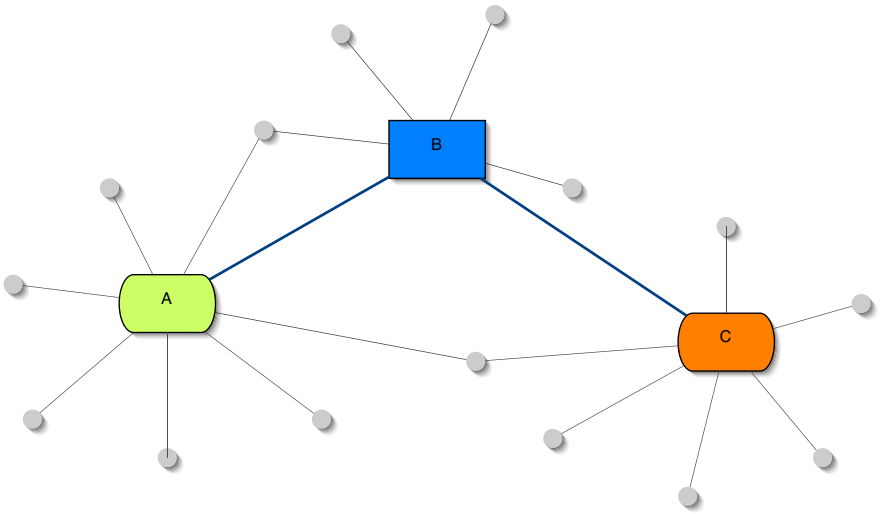

Figure 1: An example for a (very small) generated subgraph consisting of three expanded nodes, each with it's indicated neighbors and two indirectly visualized paths.

The main points that have to be looked at are:

- **Starting Point**. If the concept of the user-interface is to expand neighbors, where does the first node come from? There is a need for some sort of search algorithm.
- **Indirectly visualized edges**. How should nodes and edges be handled that are not explicitly expanded, but whose neighbors have been?
- **Paths**. One of the most interesting questions in graph-based structures is the question whether there are one or more connections between two nodes, and if, via which other nodes are they connected and of what type are the connections/edges?
- **Filters**. Which types of elements should be taken into account when drawing neighbors and when searching paths or nodes?

IMPLEMENTATION OF GAUSSIAN PROCESS MODELS FOR NONLINEAR SYSTEM IDENTIFICATION

K. Thompson, D.J. Murray-Smith ,
Dept. Electronics and Electrical Engineering
University of Glasgow
Glasgow G12 8QQ, UK
Phone: +44 (0)141 3305222
Email: K.Thompson@elec.gla.ac.uk, D.Murray-Smith@elec.gla.ac.uk

The Gaussian Process Prior model (GP) is a non-parametric approach to Nonlinear System Identification where empirical data is analysed through the use of a statistical Bayesian framework. The GP model has been shown to provide accurate predictions of nonlinear system behaviour together with a measure of the uncertainty over each prediction. This uncertainty or variance term has been shown to be of particular value in the design of adaptive or predictive controllers where the behaviour of a control system may be modified to reflect the uncertainty associated with the prediction.

The GP model may be considered as a 'black-box' method as the identification process relies solely upon experimental data. However, the inclusion of prior system knowledge into the modelling procedure can provide valuable insights as to the worth of the recorded data and effectiveness of the resultant model, especially when dealing with real systems where data may be limited. Previous research into modelling with GPs has concentrated more upon the mathematical methodology and theoretical possibilities of the approach, with the issues regarding the implementation of the GP approach yet to be fully explored. This work aims to demonstrate the practicalities of the approach and when applied to simple simulated systems displaying 1^{st} and 2^{nd} order nonlinear characteristics.

Although variants of the GP model have been successfully employed in various formats over the years towards the problem of modelling static nonlinearities and statistical classification, research carried out recently by Girard et al [1] and Kocijan et al [2] has sought to adapt the GP approach toward the goal of modelling nonlinear dynamic systems.

The overall approach taken by the GP model is to utilise a set of noisy training data, consisting of recorded system input and output values, with which to infer new output predictions given a set of new test input. For this to be achieved, the objective of the GP process is to assign the function to be identified, f(x), a prior probability density function. The prior distribution (based upon the training data) will then be used to find the predictive distribution of y_{n+1} from new input data x_{n+1}. The GP prior is a collection of random variables that are assumed to have a joint multivariate Gaussian distribution allowing it to be fully specified by its mean μ and covariance Σ.

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IMPROVING THE LOCAL MODELLING OF THE CHAOTIC TIME SERIES

M. Ataei
The University of Isfahan
Hezar-jarib Ave., 81744, Isfahan, Iran
Phone: +98 311 7933050 Fax: +98 311 7933071
Email: Ataei@eng.ui.ac.ir or mataei1971@yahoo.com

Abstract. The chaotic behaviour has been appeared in many disciplines like engineering and physical sciences and in most of them only a scalar or vector sequences of measurements are available in the form of time series. As another fact, scientists and engineers rely on models to understand the particular process, to make predictions, to control its dynamics, and to reduce the noise. Moreover, the model of chaotic time series can be used also in calculating the Lyapunov exponents and the attractor dimension, which are useful dynamical diagnostic for deterministic chaotic systems. Therefore, techniques for constructing models that are based on time series data have drawn the attention of many researchers and various techniques have been investigated.
Generally, in a deterministic system, the model describes the evolutionary equation in which the future value is considered to be dependent to past and present values and this relation is described by a map. The free parameters in this predictive map are optimized by minimizing a definite cost function. There are different model classes which generally can be considered in two approaches: global methods, and local methods. In global modelling we have to choose an appropriate functional form of map which is flexible enough to model the true function on the whole attractor of the chaotic system and is applicable when the dynamics of system is sufficiently smooth [1]. In contrast with global approach, if the time series of output measurements is long and the noise level is small, local method can be effective which is simpler than global models but may require more numerical computations. In this approach, it is tried to fit a local function which maps the phase space points in a neighbourhood to their images. The use of local models for prediction has been accomplished in some references, e.g. [2-3]. They can be used in other time series analysis like estimating the Lyapunov exponents [4]. A vexing problem in constructing the local model is the appropriate choice of the values of the model parameters such as the model order and size of the neighbourhood. Some methods for optimizing the size of neighbourhood, the embedding dimension and the distance metric are described in [5, 6].
In this paper, two important factors in local modelling which any modification in them causes improvement in final model are considered. These parameters are suitable local model order and correct neighbourhoods. The model order is related to the minimum number of differential equations which is required to describe the steady state process. This number is closely related to the dimension of strange attractor; however it should be distinguished from global embedding dimension. In this paper a method for estimating the order of local model is presented. This is accomplished by checking the property of no self-intersection of the trajectories in the reconstructed state space. In other words, if all the neighbour points in m-dimensional space are also neighbours in $(m+1)$-dimensional space, then the minimum value of m can be considered as the suitable model order.
The other factor is the selection of true neighbours and appropriate number of neighbours which is important in the estimation of the unknown coefficients of the model. The number of neighbours should also be determined with some considerations on the local neighbourhood selection. To show the improvement due to the proposed methodology, the analysis of a well known chaotic system in order to estimate its Lyapunov exponents from available time series of its measurements is considered. It is shown that the proposed procedure results in the actual dimension of local model which improves the local modelling and finally make improvement in chaotic system analysis.

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IDENTIFICATION AND APPROXIMATION OF RATIONAL AND NON-RATIONAL LINEAR CONTINOUS TIME SYSTEMS

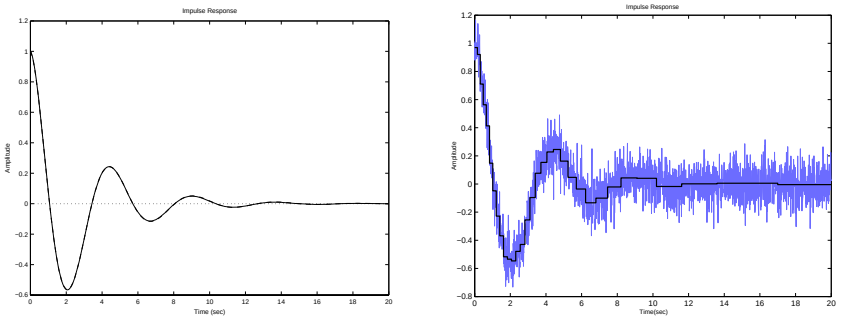
U. Konigorski, TU Darmstadt, Germany

Darmstadt University of Technology
Landgraf-Georg-Strasse 4, D-64283 Darmstadt, Germany
Phone: +49 6151-16-3014, Fax: +49 6151-16-6114
email: ukonigorski@iat.tu-darmstadt.de

In various fields of modelling and control non-integer differentiation has proven to be an adequate mathematical concept to describe physical effects like damping, diffusion etc. In case of linear systems this leads to non-rational transfer functions in the Laplace domain [1]. This paper presents a new unified approach for identification and approximation of rational as well as non-rational and transcendental systems which is based on an algebraic representation of linear continous time systems.

As with classical linear time invariant LTI-systems all of these systems can be described by a transfer function $G(s)$ in the Laplace domain. In case of fractional order systems beside rational polynomials the corresponding transfer function also exhibits non-integer powers of the Laplace variable s. Moreover, modelling of linear distributed parameter systems usually results in transcendental terms in $G(s)$.

Up to now a lot of different approaches for identification, approximation and order reduction of linear systems have been proposed in the literature. Some of them are based on discrete time system representations while others rely on a continous time description. Meanwhile there also exist several methods which allow for identification of non-rational systems [2]. In what follows a new unified approach for linear continous time system identification and approximation is presented which covers all kinds of linear continous time systems, i.e. all linear systems with a transfer function $G(s)$. This approach is based on an algebraic representation of linear continous time dynamic systems presented in [3]. This representation yields the linear relation $\overline{\mathbf{g}} = 2\alpha\mathbf{L}^{-1}\mathbf{g}(\alpha)$ between the stairstep approximation $\overline{\mathbf{g}}^T = [g_0, \ldots, g_{N-1}]$ of the system's impulse response (see figure 1(b)) and the N values $\mathbf{g}^T(\alpha) = [G(2\alpha), \ldots, G(2N\alpha)]$ of its corresponding transfer function $G(s)$ in the Laplace domain and is based on a Fourier series approximation of linear systems by means of Walsh functions. The parameter α results from a nonlinear time transformation and can be used to account for the global systems dynamics, e.g. the settling time of the system.



(a) (b)

Fig. 1: (a) Impulse responses of the fractional oscillator $X(s) = \frac{s}{s^2+s^{0.5}+1}$ (—) and its rational approximation $\hat{X}(s) = \frac{0.3167s^3+1.4246s^2+0.7842s+0.0066}{0.3158s^4+1.4783s^3+1.9842s^2+2.8180s+1}$ (- - -). (b) Noisy impulse response of the fractional oscillator and its numerically calculated stairstep approximation.

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LINEAR REGRESSIVE MODEL STRUCTURES FOR ESTIMATION AND PREDICTION OF COMPARTMENTAL DIFFUSIVE SYSTEMS

Corresponding author: D. Vries
*Dept. of Agrotechnology and Food Sciences, Systems and Control Group,
Wageningen University, The Netherlands
Phone: ++31 317 482 014, Fax: ++31 317 484 957
†Dept. of Applied Mathematics, Faculty of EEMS, University of Twente
The Netherlands

D. Vries*, K.J. Keesman*, H. Zwart†

In input-output relations of (compartmental) diffusive systems, physical parameters appear non-linearly, resulting in the use of (constrained) non-linear parameter estimation techniques with its short-comings regarding global optimality and computational effort.

Our approach is to handle the parameter estimation and prediction problem, initially for an LTI infinite-dimensional system, via discretization and a linear regressive parametric realization of the system in order to obtain unique estimates. However, unlike a black box 'data based' approach such as subspace identification, we will conserve the physical compartmental model structure due to the reasons mentioned before.

In particular, we will consider a set of finite LTI state space systems which can be regarded as compartmental diffusive systems. By the properties of such a system (denoted as Σ^d), we are able to find another realization of Σ^d which is suited for linear regressive estimation and prediction. After some integral transform of Σ^d, we obtain a set of linear equations of the form $\varphi^T M\psi = b$. It will be shown, that the inverse of M is the resolvent of the system matrix A in Σ^d. In the specific case that A is a symmetric tridiagonal matrix, explicit solutions for the inverse of M are known. The key here is to find M^{-1}, such that we may rewrite this as a linear regressive set of equations: $\theta^T\phi = \gamma$, with $\theta = \xi(\vartheta)$ a known reparametrization function of the physical parameter ϑ. From hereon, it is rather straightforward to arrive at an estimate $\hat{\theta}$ using existing estimation techniques. By a rearrangement of terms we get an explicit expression for the output at time instant k, *i.e.* $\hat{y}(k|\hat{\theta}; Z^-)$ with Z^- the current available input-output data set.

The key objectives of the paper are defined as follows:

(i) to show the procedure to obtain a linear regressive *mechanistic* (or also referred to as physical) model representation, say $\Sigma^{\mathrm{LR}}(\phi, \gamma)$ from a linear state space model $\Sigma(A, B, C, D)$

(ii) to show the application of approach (i) to

Case A a (finite) compartmental approximation of a boundary control system with Dirichlet boundary conditions, and,

Case B a (finite) compartmental approximation of a boundary control system with one Neumann boundary condition

(iii) to show some estimation results of one case, that is, Case A.

For two compartmental diffusive models we have derived linear regressive structures suitable for linear regressive estimation and prediction. For one case, we illustrate the strength of linear regressive estimation by a simulation study. Simulation of Case A with added disturbances to the output, indicates that the sketched methodology is attractive for linear regressive estimation and prediction. Furthermore, since we keep track of the physical parameters, physical knowledge in the model structure is preserved throughout analysis and estimation.

An approximate normal form approach to sampled representations of nonlinear systems

Joachim Deutscher, Universität Erlangen-Nürnberg, Germany
Lehrstuhl für Regelungstechnik, Universität Erlangen-Nürnberg
Cauerstraße 7, D–91058 Erlangen, Germany
Phone: + 49 (0)9131/85-27128, Fax: + 49(0)9131/85-28715
email: joachim.deutscher@rt.eei.uni-erlangen.de

This paper considers the time discretization of nonlinear continuous time systems. If one is interested in a sampled system that reproduces the samples of the continuous time system exactly, then an initial value problem for a nonlinear differential equation has to be solved within the sampling interval. One approach to solve this problem is to expand the solution in a Taylor series which yields a Taylor-Lie series representation of the sampled system (see [KK97, MNC85]). Since in practical applications only a truncation of the Taylor-Lie series can be considered, the resulting sampled system is only accurate for sufficiently small sampling periods. However, in many practical applications it is desirable to use large sampling periods due to the available machine time. This can be achieved by computing an approximation of the nonlinear continuous time system that admits a closed form solution of the initial value problem.

The aim of this paper is to compute exactly discretizable approximations of nonlinear continuous time systems. In order to enlarge the domain where the corresponding discrete time model is valid not only the linear part but also higher order terms of the Taylor expansion of the continuous time system are taken into account. This is achieved by calculating a nonlinear change of coordinates that transforms the Taylor expansion of the continuous time system into a polynomial triangular form for which a closed form solution of the initial value problem exists. On the basis of this solution a closed form sampled representation of the nonlinear system with solely finite degree polynomial nonlinearities can be obtained. For computing the change of coordinates a normal form approach is proposed that transforms the terms of the Taylor expansion of the continuous time system into triangular form step by step (see e.g. [TR02]). The benefit of this procedure is that in each transformation step only a set of linear algebraic equations has to be solved which can easily be implemented using a numerical software package. If these equations are not solvable a least square solution is computed. As a consequence the resulting exactly discretizable triangular system approximates the nonlinear system in the new coordinates in the least square sense. Since calculating the sampled representation by direct integration of the triangular system may be rather tedious an alternative time discretization procedure for triangular systems is presented. It is shown that every triangular system can be exactly embedded as a bilinear system in a higher dimensional state space. For the resulting bilinear system a solution of the initial value problem exists in form of matrix exponentials that can be evaluated symbolically for sufficiently small system orders. If this is not possible a numerical procedure for computing the sampled system is proposed. To this end, expressions are derived for the coefficients of the polynomial nonlinearities of the sampled system that can be calculated numerically. The sampled representation of the triangular system can be obtained from the sampled representation of the bilinear system by simply omitting difference equations such that it has the same order as the original continuous time system. A simple example is used to demonstrate the new discretization approach.

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Multiscale Modelling in Materials Science

MULTI-SCALE APPOACHES IN COMPUTATIONAL MATERIALS SCIENCE

P. Weinberger, Vienna University of Technology, Austria

Corresponding Author: P. Weinberger
Vienna University of Technology
Getreidemarkt 9/134, 1060 Vienna, Austria
email. pw@cms.tuwien.ac.at

The term "multi-scale" is presently very much *en vogue*, one almost gets the impression that this term very often is simply used to emphasize the "importance" of a particular scheme or to impress an audience with a "buzz word". In the applied mathematics literature [1] it seems that essentially two types of multi-scale schemes are in discussion, namely "one shot" schemes in which one approach is combined in a consecutive manner with another one of different mathematical origin, and procedures by intertwining two such approaches "iteratively", or, to use a term more common in physics and chemistry, "selfconsistently".
Clearly enough the easiest way to define multi-scale procedures in particular in the realm of physics and chemistry would be to state that a combination of say two different kinds of differential equations is required. Although this in principle would be a valid definition it is too narrow, since, e.g., any use of density functional theory (DFT) requires already the application of two differential equations of different kind, namely the Kohn-Sham equations (effective Schrödinger or Dirac equation) and the Poisson equation, in an "iterative" manner. Surely enough nobody would call *abinitio* type calculations in terms of the DFT a "multi-scale" procedure. This simple counter-example indicates that it is perhaps quite appropriate to discuss the concept of "multi-scale" only in the context of a particular field of research or discipline. In the present paper such a discussion is devoted to computational physics, in particular to computational materials science, since this is a well-established field of research in which many different types of computer simulations are performed.

Formal distinctions

Suppose multi-scale schemes refer to a combination of different levels in physics such as, e.g., by combining quantum mechanical approaches with phenomenological ones, or, phrased differently, by combining microscopical with macroscopical schemes. A "one shot" multi-scale procedure would then consist of a quantum mechanical calculation (e.g., within the framework of the DFT) followed by a phenomenological one, in which the results of the former are used; an "iterative" procedure combines both in a kind of selfconsistent manner [2 – 7]. In the latter case of course great care has to be taken that fundamental concepts are not violated (microcosmos versus macrocosmos), i.e., that only quantities can be varied that are well-defined on both "conceptual" levels.
Two typical situations will be discussed, namely augmenting a time-independent quantum mechanical scheme with (1) the concept of time (e.g., in terms of the phenomenological Landau-Lifshitz-Gilbert equation), and (2) with a method typical for statistical mechanics (e.g., Monte Carlo simulations based on ab-initio determined parameters), both schemes in fact can be operated in an iterative manner. Most frequently in computational materials science "one-shot" multi-scale procedures are used, in which typically physical properties of materials are calculated in terms of the results of *ab-initio* approaches. In order to be classified as a multi-scale approach the evaluation of these properties has to be based on a scheme, which by definition is different from a typical DFT method such as, e.g., the Kubo equation for evaluating electric and (magneto-) optical transport, i.e., by requiring “physically separate” computer program packages that in the end provide macroscopic quantities. Very often also multiple combinations of "one shot" multi-scale procedures are used as for example in evaluating magnetic domain wall properties [8 – 10], the switching times (pico-second regime) in current induced switching [11 – 13], or, rotation and ellipticity angles in the magneto-optical Kerr-effect [14 – 16].

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NEW SCALES: PROPERTIES OF NANOSTRUCTURES IN THE FEMTOSECOND REGIME

A. Vernes, P.Weinberger, Center for Computational Materials Science, Technical University Vienna

Corresponding Author: A. Vernes
Center for Computational Materials Science
Gumpendorfer Str. 1a, 1060 Wien, Austria
Email: av@cms.tuwien.ac.at

Many fundamental processes in matter like electron–electron or electron–phonon scattering in solids, occur on a time scale ranging from a few tenth of a femtosecond (1 fs = 10^{-15} s) to a picosecond (1 ps = 10^{-12} s). These ultrafast phenomena are experimentally accessed by monitoring the interaction of ultrashort light pulses with a given sample. Among the experimental techniques available nowadays, the so–called pump–probe methods are most frequently used. In such a pump–probe experiment one needs two ultrafast laser pulses: a pump pulse, which excites the investigated system and a probe pulse, delayed in time, which explores the relaxation of the excited system.
Based on the superposition principle of electromagnetic fields, within the Slowly Varying Envelope Approximation (SVEA) the total external electric field in a pump–probe experiment is given by:

$$\vec{E}(\vec{r},t) = \vec{E}_{pu}(\vec{r},t) + \vec{E}_{pr}(\vec{r},t)\vec{e}_{pu}\varepsilon_{pu,0}\tilde{\varepsilon}_{pu}(t)\exp\left[i(\vec{q}_{pu}\vec{r} - \omega_{pu}t)\right] + \vec{e}_{pr}\varepsilon_{pr,0}\tilde{\varepsilon}_{pr}(t-\tau)\exp\left[i(\vec{q}_{pr}\vec{r} - \omega_{pr}t)\right],$$

where $\tilde{\varepsilon}_{pu}(t)$ and $\tilde{\varepsilon}_{pr}(t)$ are the time–dependent envelopes of the pump and the probe pulse propagating in the directions $\vec{q}_{pu}$ and $\vec{q}_{pr}$ with the carrier frequencies ω_{pu} and ω_{pr} and having the polarizations $\vec{e}_{pu}$ and $\vec{e}_{pr}$. In considering an external electric field as defined in Eq. (1), it is assumed that no significant overlap in time exists between the pump and probe pulse, i.e., all coherence coupling effects can be neglected.

Generalized Kubo Theory:
Because in Eq. (1) a possible overlap between the pump and probe pulse is neglected, it can be considered that for t > τ the probe pulse interacts only with the pump–excited system. The problem to be solved reduces therefore in finding the dynamic linear response of the pump– excited system with respect to the probe pulse at times t > τ. If within the interaction picture the only source of perturbation is the probe pulse then from the linearization of the density, were the density for the pump-excited state is written

$$\rho_{pr}(t) \cong \rho_{pu}(t) + \frac{i}{\hbar}\int_{\tau}^{t} dt' \quad \left[\vec{r}(t'), \rho_{pu}\right] \quad \vec{E}_{pr}(t'), \text{ and } \rho_{pu} \cong p_0 + \frac{i}{\hbar}\sum_k \int_{-\infty}^{\tau} dt \quad \left[\vec{r}(t), \rho_0\right] \quad \vec{E}_{pu}(t) \equiv \rho_{pu}^{(0)} + \rho_{pu}^{(1)}$$

Accordingly the frequency–frequency representation of the generalized, strictly linear conductivity or the pump–probe experiments is given by ref[1]:

$$\tilde{\sigma}_{\mu\nu}^{(0)}(\omega_{pr},\omega;\tau) = \frac{1}{2\pi}\exp\left[+i(\omega-\omega_{pr})\tau\right] \quad \mathcal{L} \quad \left[\tilde{\varepsilon}_{pr}(t)\right]_{i(\omega_{pr}-\omega)}\tilde{\sigma}_{\mu\nu}(\omega) \qquad [2]$$

where in terms of ω this quantity is now resolved with respect to the spectral components of the probe pulse. The first order conductivity, on the other hand, is resolved with respect to he spectral components of the pump pulse and hence is written as (ref.[1])

$$\tilde{\sigma}_{\mu\nu}(\omega_{pr},\omega_{pu},\omega;\tau) = \frac{\beta}{2\pi}\exp\left[+i(\omega-\omega_{pu})\tau\right]\sum_k \varepsilon_{pu,0k}\int_0^{\infty} dt\exp(+i\omega t) \int_0^{t} d\xi\tilde{\varepsilon}_{pr}(t-\xi)\exp(i\omega_{pr}\xi) \int_0^{\infty} d\xi'\left\langle J_{\mu}(t), J_{\nu}(t-\xi), J_K(-\xi')\right\rangle\tilde{\varepsilon}_{pu}(\tau-\xi')\exp(+i\omega_{pu}\xi'). \qquad [3]$$

Although for this form one can also take advantage on the properties of Laplace transforms, for $\sigma_{\mu\nu}^{(1)}(\omega_{pr}\omega_{pu}\omega;\tau)$ a similar expression to that in Eq. (2) cannot be deduced. The total and normally linear dynamic conductivity is finally obtained by combining the zeroth and first order conductivities as given by Eqs. (2) and (3),

$$\tilde{\sigma}_{\mu\nu}(\omega_{pr},\omega_{pu},\omega;\tau) = \tilde{\sigma}_{\mu\nu}^{(0)}(\omega_{pr},\omega;\tau) + \tilde{\sigma}_{\mu\nu}^{(1)}(\omega_{pr},\omega_{pu},\omega;\tau).$$

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Scientific computing in thin film growth

Axel Voigt,

research center caesar
Ludwig-Erhard-Allee 2
53175 Bonn
Deutschland
voigt@caesar.de

A Model Hierarchy for Surface Diffusion: The Small Slope Case

Martin Burger

Industrial Mathematics Institute, Johannes Kepler University
Altenbergerstr. 69, A 4040 Linz, Austria
martin.burger@jku.at

Abstract

Surface evolution and its mathematical modelling is a field of high importance for various applications, in particular for growth processes in materials science. A growth mode of particular interest for many modern technologies is *surface diffusion*, which appears to be the dominating process in nanosurface growth.

This paper provides an overview of some recently developed models for the evolution of interfaces (in particular thin films) by surface diffusion mechanisms. We shall put these models into a hierarchy, and study their relation in detail for a small slope approximation. The starting point is a model including explicit diffusion equations for the adsorbed particles along the evolving surface, which we scale and investigate model reductions for small- and large-parameter asymptotics. In this way we establish connections between some well-known models and also obtain some new intermediate models in certain cases.

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Stochastic Optimization Models

ENDOGENOUS RISKS AND LEARNING IN CLIMATE CHANGE DECISION ANALYSIS

B.C. O'Neill, Y. Ermoliev and T. Ermolieva
International Institute for Applied Systems Analysis

Corresponding Author: Brian C. O'Neill,
International Institute for Applied Systems Analysis (IIASA)
Schlossplatz 1, A-2361 Laxenburg, Austria
Phone: +43 2236 807 0, Fax: + 43 2236 71313
email: oneill@iiasa.ac.at

Discussions of climate change policies are often framed as a choice between acting now or waiting until we know more about the problem. The climate change policy dilemma poses a "hit-or-miss" type of decision making situation. Emissions of greenhouse gases (GHG) are associated with the production and consumption of goods and services, and the atmospheric concentration (stock) of these long-lived pollutants may cause irreversible damages. On one hand, postponing the reduction of GHG emissions may lead to potentially irreversible climate-related impacts, for example, reorganizations of large-scale ocean circulation patterns or increased frequency of extreme weather-related events. On the other hand, if the problem turns out to be less severe than expected, the delay will avoid irreversible investments in capital for emissions abatement.

In this paper we take a different approach. Instead of using expected damages we explicitly introduce safety constraints by formulating the climate change problem within the framework of stabilization. We first characterize climate change risk by the probability of total atmospheric CO2 concentrations exceeding a vital random threshold associated with potential ranges of global temperature. We outlines a two-stage dynamic climate change stabilization STO model with random durations of stages. In general, this model can be solved only numerically and therefore the key factors driving results are difficult to identify. For these reasons, we analyze only stylized aspects of the model; these provide a clearer picture of the various driving forces and show why the ability to learn in the future can lead to either less-restrictive or more-restrictive *ex ante* abatement policies today.

Next, we use a very simple linear two-stage STO model to illustrate that the results from empirical models can be rather contradictory, because optimal solutions depend on complex non-smooth interactions among *ex ante* and *ex post* decisions, costs, and probability distributions. In particular, they induce potentially strong risk aversion characterized by risk measures that are used for regulating the safety of nuclear plants and insolvency of insurance companies, but also in financial applications, extremal value theory [1], and catastrophic risk management [2].

We then analyze the effects of uncertain costs and random duration of stages. This analysis emphasizes the importance of quantiles of probability distributions characterizing key uncertainties and shows that without aggressive *ex ante* commitments, a misperception of limited adaptive second-stage capacity may provoke a catastrophe (i.e., exceedance of the safety constraint). We also discuss the controversial effects of incomplete learning and nonlinear costs, which more strongly and even unconditionally require coexistence of *ex ante* anticipative and *ex post* adaptive risk-management decisions. Finally, a more realistic but still linear dynamic two-stage climate change stabilization STO model is analyzed. The explicit incorporation of *ex ante* and *ex post* decisions induces risk aversions characterized by a dynamic version of a CVaR-type risk measure. This may create a wrong impression of truly risk-based policy analysis and, without explicit introduction of adaptive capacity and additional safety constraints, may provoke a catastrophe.

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AN INTEGRATED APPROACH TO CATASTROPHIC RISKS MANAGEMENT

G. Fischer, T. Ermolieva, H.T. van Velthuizen
International Institute for Applied Systems Analysis,
Laxenburg, Ausrtia

Corresponding Author: G. Fischer,
International Institute for Applied Systems Analysis
Schlossplatz 1, A-2361 Laxenburg, Austria
Phone: (+43 2236) 807 292, Fax: (+43 2236) 807 533
email: fisher@iiasa.ac.at

The main reason for ever increasing losses from human-induced and natural catastrophes is inappropriate land use practices, clustering of industries, people, and capital in hazard-prone areas as well as arising of new hazard-prone areas, a phenomenon that largely attributes to the lack of knowledge of the risks. Analysis of insurance companies by Froot [4] shows that because of economic growth in hazard-prone areas, damages due to natural catastrophes alone have grown at an average annual rate of 5 percent. Locations may be subject to disasters which may be unlike anything that has been experienced in the past. Therefore, it is impossible to improve policies by relying only on historical databases or to use "learning-by-accident" approach. For all these reasons, the use of models becomes essential (see [1], [2], [5] and references therein).

This paper presents a general integrated catastrophic risk management model developed at IIASA for case studies of seismic, flood, windstorms, and livestock epidemics risks. The model accounts for the specifics of the risks: severe dependent losses, scarcity of historical information on occurrences of catastrophes at particular locations, the need for long-term perspectives and geographically explicit analyses.

We show that the design of strategies against catastrophes can be viewed as a spatial and dynamic stochastic optimization problem combining goals and constraints of such agents as producers, individuals, governments, insurers, reinsurers, investors. We propose Monte Carlo-based optimization methods allowing to deal with essential computational complexities of the problems and specific rebalancing procedures [3] for downscaling of aggregate data. The model bridges decision oriented economic theory with risk theory and catastrophe modeling. Risk management decisions are evaluated from the long-term perspectives of the welfare growth in a region showing that financial reserves and land use strategies for catastrophes management should be properly evaluated over years. The implication of extreme events on the proper choice of discounting is illustrated.

The proposed model and methods are illustrated by flood risks case study on Tisza river in Hungary and Ukraine [3]. For these countries, facing special problems of a poor and immobile population, ex-ante land use strategies for risk mitigation and the establishment of a multipillar flood loss-sharing program, are especially important.

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DISCOUNTING, CATASTROPHIC RISKS MANAGEMENT AND VULNERABILITY MODELING

Y. Ermoliev, T. Ermolieva, G. Fischer, S. Nilson, M. Obersteiner

International Institute for Applied Systems Analysis,
Laxenburg, Ausrtia

Corresponding Author: Y. Ermoliev,
International Institute for Applied Systems Analysis
Schlossplatz 1, A-2361 Laxenburg, Austria
Phone: (+43 2236) 807 292, Fax: (+43 2236) 807 208
email: ermoliev@iiasa.ac.at

The vulnerability of complex coupled human-environmental systems essentially relies on discounting future losses and gains to their present values. These evaluations are used to justify catastrophic risks management decisions which may turn into benefits over long and uncertain time horizons. The misperception of proper discounting rates critically affects the evaluation and may delay or provoke catastrophes. The lack of proper evaluations may dramatically contribute to increasing the vulnerability of our society to human-made and natural disasters [1]. The analysis of floods that occurred in the summer of 2002 across central Europe [3] shows that the potential areas of vulnerability to extreme events have multiplied as a consequence of failed land use and development planning. A challenge is that an extreme event, say a once-in-300-year flood, may have never occurred before in a given region. Therefore, purely adaptive policies relying on historical observations provide no awareness of the risk although, a 300-year flood may occur next year. For example, floods in Austria, Germany and Czech Republic in 2002 were classified [14] as 1000-, 500-, 250-, and 100-year events.

This paper analyzes the implications of potential catastrophic events on the choice of discounting for long-term vulnerability modeling and catastrophic management. In particular, it argues the advantages of using undiscounted random criteria allowing to properly match random horizons of potential catastrophic scenarios. It is shown that discount factors can be linked to irreversible "stopping time" extreme ("killing") events, which define the internal discount-related random horizon of evaluations. The expected duration of this horizon for standard discount rates obtained from capital markets does not exceed a few decades and, as such, these rates can not match properly evaluations of 1000-, 500-, 250-, 100- year catastrophes. We show that a typical set of such events induces declining discount rates that are asymptotically dominated by least probable events. These induced internal discount rates are conditional on the degree of social commitment to mitigate risk. In general, catastrophic events affect discount rates, which alter the optimal mitigation efforts that, in turn, change events. It is shown that this endogeneity of discounting calls for using equivalent undiscounted random evaluations, spatio-temporal vulnerability modelling, and stochastic optimisation methods.

Examples from integrated climate change modelling, flood management programs, and risky investments illustrate how the misperception of traditional exogenous discounting may provoke catastrophes and increase the vulnerability. The proposed approach allows to avoid this by using undiscounted random criteria and endogenous discounting associated with random horizons of explicitly treated potential catastrophic events. This approach critically relies on Monte Carlo based stochastic optimization.

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ADOPTION OF NEW TECHNOLOGY: THE CASE OF FUTURE PULP AND PAPER MILLS

Zuzana Chladná[1,2], Miroslav Chladný[3], Kenneth Möllersten[1,4], and Michael Obersteiner[1,5]

[1] International Institute for Applied Systems Analysis, Schlossplatz 1, A-2361 Laxenburg, Austria
[2] Department of Economic and Financial Models, Comenius University, 84248 Bratislava, Slovakia
[3] Department of Computer Science, Comenius University, 84248 Bratislava, Slovakia
[4] Department of Mechanical Engineering, Luleå University of Technology, SE-971 87 Luleå, Sweden
[5] Department of Economics, Institute for Advanced Studies, Vienna

Corresponding author: Zuzana Chladná, chladna@iiasa.ac.at

Abstract

The investment timing problem is one of the central issues in corporate finance. Although the economic evaluation of the investment is originally based on the static cash flows analysis, in this paper we lay stress on the real options techniques, which have been recognized as a proper tool for making strategic investment decisions under uncertainty (see, e.g, Dixit and Pindyck 1994). We apply the real options approach to analyze the commercial potential of CO_2 capture and storage technology applied in the pulp and paper industry (Möllersten, 2004). Our analysis is beyond the simplistic models traditionally analyzed: we attempt to implement into the model a wide class of the options in order to allow for the full flexibility in the investment process. Such a consideration requires us to construct a multidimensional binomial tree. The results of the numerical analysis are presented such that the main objective is given on the expected time when it is optimal to start with the CO_2 storage. We also explore the present value (NPV) valuation approach and compare with the optimal strategies based on the real options approach.

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Structured Modeling for Efficient Treatment of Uncertainty in Complex Problems

Marek Makowski

International Institute for Applied Systems Analysis,
Schlossplatz 1, A-2361 Laxenburg, Austria
marek@iiasa.ac.at, http://www.iiasa.ac.at/∼marek

This paper deals with two types of problems for which there are no established modeling methods and tools: first, proper treatment of endogenous uncertainty, and adequate modeling of spatial and temporal heterogeneity; second, methodology for development and analysis of models built to support analysis and solution of complex problems.

The paper presents an overview of the modeling needs and the state-of-the-art, and shows the limitations of traditional modeling methods and general-purpose modeling tools developed to deal with one of the standard problem-types through a particular modeling paradigm. The modeling requirements demand a qualitative jump in modeling methodology: from supporting individual modeling paradigms to supporting a *Laboratory World* in which various models are developed and used to learn about the modeled problem in a comprehensive way. Such a Laboratory World requires integration of various established methods with new (either to be developed to properly address new challenges, or not yet supported by any standard modeling environment) approaches needed for an appropriate (in respect to the decision-making process, and available data) mathematical representation of the problem and ways of its diversified analyses. Therefore, to be able to adequately meet the demand for advanced modeling support one indeed needs to develop and apply novel modeling methodologies. More detailed arguments (including an overview of the standard modeling methods and tools) supporting this statement are available in [1, 2].

The paper outlines the advances in three areas of modeling methods and tools:
- Structured modeling supporting the whole modeling cycle of complex problems by interdisciplinary teams working at distant locations.
- Proper treatment of irreducible uncertainty, catastrophic risks, spatial and temporal heterogeneity, downscaling, and discounting.
- Methodology and tools for integrated model analysis aimed at combining the capabilities of different methods (such as various types of simulation, optimization, multicriteria model analysis, sensitivity analysis) with data mining technology.

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MULTIPLE FIRST ORDER RELIABILITY METHODS (MFORM)

K. Marti
Aero-Space Engineering and Technology
Federal Armed Forces University Munich, D-85577 Neubiberg/Munich, Germany
Phone: +49 89 6004 2541/2560, Fax: + 49 89 6004 4641/4092
e-mail: kurt.marti@unibw-muenchen.de
WWW: http://www.stoch.net

Having to take into account in structural analysis and optimal structural design stochastic variations of the vector $a = a(\omega)$ of model parameters, the reliability of the structure is evaluated by means of the probability of survival/failure of the whole structural system or of certain relevant components. For the computation of the probability of survival p_s, an appropriate (limit) state or performance function $s^* = s^*(a, x)$ is needed to describe safe/unsafe stress states: A safe (stress) state exists if and only if $s^* < 0$, and a safe stress state cannot be guaranteed if and only if $s^* \geq 0$. The state function s^* depends on a and the vector of design variables x. The computation of p_s or the failure probability p_f is often based on a pure numerical evaluation of the state function. However, the computation of p_s can be simplified considerably if an explicit representation of $s^* = s^*(a, x)$ is available, as in the analysis and design of mechanical structures, where the state function $s^* = s^*(a, x)$ can be represented by the minimum value function of a certain convex or linear optimization problem. Standard "FORM" (First Order Reliability Method) approximation techniques are based on a linear approximation of the failure domain (in z–space) $B_{f,x}$ at a β-point z_x^*. Here, the random vector of physical model parameters a is transformed first to a standard normal distributed random vector $z = z(\omega)$. The beta-point z_x^* is the projection of the origin 0 in z–space to $B_{f,x}$. Thus, the basic reliability condition $p_s \geq \alpha_s$ can be represented by $\|z_x^*\| \geq \Phi^{-1}(\alpha_s)$, where α_s is a prescribed minimum probability and Φ denotes the cdf of $N(0, 1)$.

In order to improve the probability approximation, besides linearization of s^* at the special boundary point z_x^*, further approximations of the failure, survival domain are considered at other boundary points $b_{c,x}$ which can be obtained by minimizing/maximizing a linear form $L(z) = c^T z$, with a certain vector c, on the transformed failure or survival domain. Probability approximations of several degrees of accuracy are obtained then by considering single or joint constraints obtained by linearizing the state function $s^* = s^*(a, x)$ at the boundary points $b_{c^j,x}, j = 1, \ldots, J$, with given vectors $c^1, \ldots, c^J$. While single constraints lead immediately to explicit approximations of $p_s(x)$, for joint constraints a second approximation step is needed, based e.g. on certain Tschebyscheff inequalities. The remaining problem is then the computation of the projection z_x^* and the boundary points $b_{c,x}$. Using the above mentioned representation of s^* by the minimum value function of a convex or linear program, *explicit* parameter optimization problems for the computation of the projection z_x^* and the boundary points $b_{c,x}$ are available. Obviously, parallel computation of the boundary points $b_{c^j,x}, j = 1, \ldots, J$, is possible.

Asymptotic trajectory matching in self-navigation of autonomous manless interceptors: A nonsearch method and a formulation of the functional optimization of the stability of random systems

E. Mamontov[1], A. Koptioug[2], M. Mångård[3], and K. Marti[4]
[1] Gothenburg University, Gothenburg Sweden; [2] Mid Sweden University, Östersund, Sweden;
[3] Saab Aerosystems, SAAB AB, Linköping, Sweden; [4] Federal Armed Forces University, Munich, Germany

Corresponding author: E. Mamontov, Department of Physics, Faculty of Science, Gothenburg University, Room 7.114, the Origo building, Kemivägen 9, SE-412 96 Gothenburg, Sweden
Phone: +46-(0)31-7723489; Fax: +46-(0)317723402; email: yem@physics.gu.se

In the field of self-navigation (SN) autonomous manless robots there is a noticeable interest to the robot-based target-interception problem. The interceptor trajectory is usually determined by search-based optimization algorithms. In contrast to this, the present work treats the interception as asymptotic trajectory matching (ATM) and introduces a nonsearch version of the ATM approach to self-navigation of autonomous manless interceptors. The method treats the interception of a target by the interceptor in terms of ATM achieved by the so-called targetal stability of the ordinary differential equation for the interceptor position. More specifically, the developed SN rule for the interceptor assures that if, at some time point, the interceptor is at the same space point as that of the target, then this location matching is preserved for all the subsequent time points. Since, however, the interceptor and target are usually located at different space points, their rapprochement in the limit case of infinite time, i.e. *asymptotic* trajectory matching, is (in addition to the above SN rule) provided by the dedicated interceptor-trajectory stability termed targetal. This stability is provided by an appropriate dependence of the interceptor acceleration on the position of the interceptor relative to the target. The above nonsearch ATM-SN method is somewhat similar to the well-known inverse-dynamics technique but noticeably differs from the latter in that it determines the interceptor control vector from the trajectory of another object, the target. A comparison with the proportional-navigation strategy is also presented. The nonsearch ATM-SN method does not evaluate successive approximations and hence requires much less computing than the search techniques. This is a highly advantageous feature of the proposed method that makes it very suitable to a series of the "intelligent"-interceptor applications including those which form one of the priority areas of the European Commission.

In a general case when parameters of the interceptor are random, i.e. the entries of a multidimensional random variable, the nonsearch ATM-SN method leads to a formulation of a new problem in stochastic optimization. It is the functional optimization of the interceptor (targetal) stability. This problem is inherently related to stability, probability theory, and optimization techniques. Moreover, it is of a specific application significance.

Another group of the new results developed in the present work is related to the sensors which can assure truly autonomous (in particular, fully GPS-free) operating of the interceptors. The work proposes the basic physical principles and schemes for the above sensors. This is a crucial contribution to a practical implementation of the corresponding interceptors. It also stresses a distinct practical ground for future development in the field.

A list of the fundamental and applied topics for future research is also suggested.

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PARAMETER ESTIMATION OF THE GENERALIZED GAMMA DISTRIBUTION

GOMES O.*, COMBES C.**, DUSSAUCHOY A.***

*PRISMa, Bât Nautibus, Université Lyon 1, 43 bd du 11 novembre 1918, 69622 Villeurbanne cedex- France - ophelie.gomes@laposte.net
**EURISE – Faculté de Sciences, Université Jean Monnet, 23 rue du Docteur Paul Michelon, 42023 Saint-Etienne cedex 2 - France - combes@univ-st-etienne.fr
*** PRISMa, Bât Nautibus, Université Lyon 1, 43 bd du 11 novembre 1918, 69622 Villeurbanne cedex- France - alain-d@bat710.univ-lyon1.fr

This article focuses on the parameter estimation of the generalized gamma distribution. Because of many difficulties described in the literature to estimate the parameters, we propose here a new estimation method. The algorithm associated to this heuristic method is implemented in Splus. We validate the resulting routine on the particular cases of the generalized gamma distribution.

The generalized gamma distribution is a younger distribution (1962) than the normal distribution (1774). It was introduced by Stacy [5] in order to combine the power of two distributions: the Gamma distribution and the Weibull distribution. The generalized gamma distribution is a popular distribution because it is extremely flexible. This distribution is also convenient because it includes as special cases several distributions: the exponential distribution, the LogNormal distribution, the Weibull distribution, the Levy distribution…
These interests are nevertheless in contradiction with the difficulties in estimating the parameters. This topic was dealt in many papers but the complexity of the results proves that this topic is still an opened item.
This paper proposes a new heuristic approach in parameter estimation of the generalized gamma distribution using an iterative method. This routine was implemented in Splus software.
In the section 2, we describe the characteristic of the generalized gamma distribution and give some application areas. An overview of literature on the parameter estimation of the generalized gamma distribution is presented in section 3. The section 4 deals with the proposed heuristic method called algorithm I.T.E.V. In section 5, we apply the resulting routine on known generalized gamma distribution in order to validate the estimation method. We terminate with a conclusion and some perspectives.

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Keywords: Shifted generalized gamma distribution, generalized gamma distribution, parameter estimation, Chisquared goodness-of-fit test.

Simulation Service Providing based on Web Service Technology with Standardised DEVS Models

M. Gyimesi, Vienna Univ. of Technolgy

Corresponding Author: M. Gyimesi
Vienna University of Technology
Argentinierstr. 8, 1040 Wien, Austria
Phone: +43 1 58801-10159
email: mgyimesi@osiris.tuwien.ac.at

Not only outstanding persons in the field of computer science underrated the upcoming importance and possibilities of computers and computernetworks – e.g. Thomas Watson, chairman of IBM in 1943 thought that "… there is a world market for maybe five computers". In the early nineties of the last century, computer networks and in particular the Internet was well established. But scarcely anybody had knowledge of Tim Berners-Lee's World Wide Web (WWW) or foresaw the importance of the WWW.
Today the internet and the WWW is on the cusp of a paradigm shift. Up to now most actions in the WWW are a sort of human-computer interaction, but the introduction of the eXtensible Markup Language (XML) changed the perception. The internet will be seen as a great space of information and with the use of XML and following technologies like Web Services, Grid Computing and Semantic Web the difference between human-machine interaction and machine-machine interaction vanishes.
Meanwhile the simulation domain not only noticed an emerging demand and development of webbased simulation but adopted the concept of Application Service Providing (ASP) from Business to Business (B2B) communication.

This work investigates the usefulness of XML in the simulation domain and uses web service technology to build the SimASP framework for discrete event simulation (DES). Figure 1 outlines the general concept of the framework.

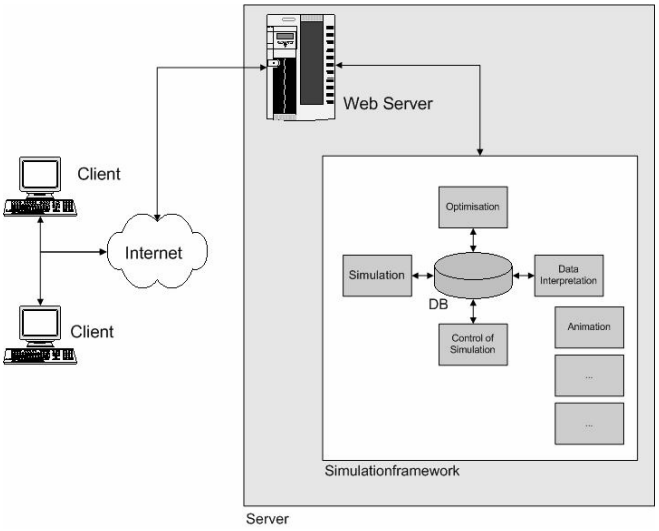

Fig. 1: The Concept of the SimASP framework

The full paper will discuss both the framework and the combination of DES with XML. The use of XML as description for DEVS models sets the basis for a standardized modeling description in DEVS models, comparable with Modelica in continuous systems modeling. An extended list of references will be given.

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An Optimisation-Oriented Model of Distributed Supply-Chain

Marco Ghirardi, Giusepppe Menga, Nicola Sacco

Department of Control and Computer Sciences - Polytechnic of Turin
c.so Duca degli Abruzzi, 10129 Turin, Italy
{marco.ghirardi,giuseppe.menga,nicola.sacco}@polito.it

In the last decades, due to the new technologies in the fields of information and telecommunication, global automation ([1]) has transferred and extended classical process control and factory automation ideas to geographically distributed environments. In this framework, Distributed Supply Chains (DSCs) result to be networks of autonomous components, operating in a competitive or cooperative environment, in which no hierarchy in decision making is enforced and where the initiatives to reach a common goal are taken by each partner.

While in the relevant literature there are many centralised approaches to the optimisation of DSC ([2]), in the era of Internet many researchers have devoted their attention to the interconnections of autonomous agents ([3]) and decentralised decision modules which are able to guarantee that no hierarchy in the decision making is enforced.

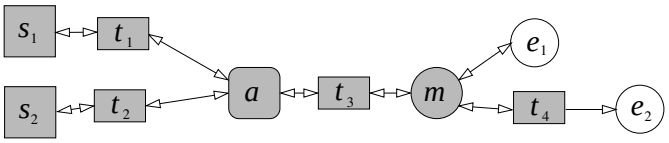

Figure 1: An example of distributed Supply-Chain.

In this framework it is worth designing suitable decentralised algorithms which are able to take advantages from the distributed architecture of the DSC. Then, to this aim, in this paper a suitable model of DSCs, as the one depicted in Fig. 1, is presented with the aim of providing a tool for DSC distributed optimisation. In particular, in the first part of the paper, a general modular modelling approach for distributed supply chains, including suppliers (s), processing units (m), assemblers (a), transportation systems (t), and external customers (e), is presented with the aim of keeping the framework as general as possible. In the second part of the paper, a brief description of the optimisation algorithms is also presented.

Thus, the main result of this work is the formalisation of an effective model for decentralised control problems which is able to take into account both the production/transportations costs of each element of the supply-chain and the cost due to earliness and tardiness of the external orders of the DSC.

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OPTIMAL PRODUCTION PLANNING IN A FIRM SUBJECT TO ENVIRONMENTAL CONSTRAINTS

Marius Rădulescu and Sorin Rădulescu
Institute of Mathematical Statistics and Applied Mathematics, Casa Academiei Române,
Calea 13 Septembrie nr.13, RO-050711, Bucharest 5, ROMANIA,
e-mail: mradulescu@csm.ro

Constanța Zoie Rădulescu
National Institute for Research and Development in Informatics, 8-10 Averescu Avenue,
011455, Bucharest 1, ROMANIA, e-mail: radulescu@ici.ro

At present the market positions of industrial firms are challenged by a trend of increasing pollution charges and environmental taxes.

Furthermore, European Directive CE 61/96 "Integrated Pollution Prevention and Control" (IPPC) requires that the industrial sectors change their production techniques according to Best Available Techniques (BAT), defined with the objective to reduce the impacts on the environment as a whole.

Various strategies have been developed to mitigate the effects of pollution. Unfortunately these strategies are expensive to implement and may take years to have the desired effect. The key is pollution prevention rather than clean up or control, although the alternative approach of source reduction may be a start to the prevention process.

Many governmental programs and policy instruments were implemented in order to reduce or to achieve certain environmental standards. The firm managers become more and more aware of the potential benefits of the integrated production-planning decision support systems.

In reality the compliance with environmental standards can only be achieved with a certain probability.

The present paper presents an original approach to the optimal production planning in a firm subject to environmental constraints.
Optimal production plans are derived for an industrial firm subject to constraints on pollution emissions. The manufacture of every product produces zero, one or several emissions. The cumulative effect of each emission must be bounded by a given threshold. Three pollution levels are defined: a target level, an alarm level and a maximum admissible level. The probability of overcome these levels must be minimized and the expected return of the production plan must be maximized. A multiobjective stochastic programming problem is formulated. The ranges of user parameters are determined. Starting from this problem are formulated a maximum expected return problem and a minimum pollution risk problem.
In the maximum expected return problem the manager tries to maximize the expected return taking into account the following restrictions:

- the probabilities that the cumulative effect of the polluting emissions overcome the pollution levels d_{sj}, s = 1,2,3 are smaller than the admissible risk degrees ε_{sj}
- the sum invested in the fabrication plan is equal to *M*.
- for all $k \in \{1,2,..., p\}$ the total amount of resource R_k required by the fabrication plan is less or equal than r_k

In the minimum pollution risk problem the manager tries to minimize a linear combination (with positive coefficients) of the probabilities of overcoming the pollution levels taking into account the following restrictions:

- the probabilities that the cumulative effect of the polluting emissions overcome the pollution levels d_{sj}, s = 1,2,3 are smaller than the admissible risk degrees ε_{sj}
- the expected return is greater than a given level *W*.
- the sum invested in fabrication plan is equal to *M*.

The case when the random vectors b_j which define the unit emission outputs have a multivariate normal distribution is studied.
A case study for a textile firm is analyzed and a numerical example is presented.

Timed Petri net simulation in Matlab: A production cell case study

Thomas Löscher[1], Dejan Gradišar[2]
Felix Breitenecker[1], Gašper Mušič[2]
[1]Vienna Univ. of Technology, Department of Analysis and Scientific Computing
Wiedner Hauptstrasse 8/101, 1040 Vienna, Austria
thomas@loescher.at, felix.breitenecker@tuwien.ac.at
[2]Univ. of Ljubljana, Faculty of Electrical Engineering
Tržaška 25, 1000 Ljubljana, Slovenia
{dejan.gradisar, gasper.music}@fe.uni-lj.si

Abstract. This paper deals with a production cell where different types of products can be processed in a given sequence. The process flow is modelled using timed Petri nets. A Matlab Petri net toolbox is used to simulate the model of the production cell. For this reason a new conflict resolution is implemented into the simulation function where priorities and sequences can be taken into the consideration. The given sequence can be evaluated with the simulation. Afterwards the results can be shown in a Gantt chart.

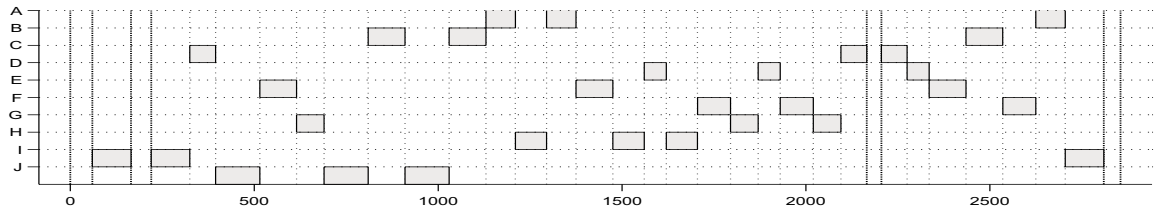
Petri nets represent a powerful graphical and mathematical modelling tool [4]. Many different extensions of classical Petri nets exist, and these are able to model a variety of real systems. In particular, timed Petri nets can be used to model and analyze a wide range of concurrent discrete-event systems [1]. Several previous studies have addressed the timed Petri-net-based analysis of discrete-event systems, including flexible manufacturing systems (FMS)[4].

In this work a simulation oriented analysis of a timed Petri net model of a production cell is presented. The analysis is performed within Matlab, a general-purpose computational environment which yields high flexibility and several presentation capabilities. To facilitate building of the Petri net models a graphical editor [3] was improved and supplemented with the capability of timed Petri net simulation.

The problem of simulation of different operational sequences in a production cell is considered. In this special type of a production cell [3] different types of products can be processed. Each product type requires a special fixture and for each type exist only one fixture. This fixture is used to fix the product into the suitable position for processing. Platforms are used to move and shift the products inside the production cell.

In this work timed Petri nets (holding duration principle [1]) with deterministic time delays are used to model the behavior of the production cell. The Petri net model is built and simulated in Matlab 7.0.1. Therefore the Matlab Petri net toolbox from [3] is adapted to Matlab 7.0.1. A new conflict resolution method is added to the timed simulation function [2]. Transitions can be selected and added to disjoint vectors. Afterwards a priority or a sequence can be specified to each vector of transitions. Usually the number of different product types is greater than the number of platforms. Therefore an algorithm is implemented to calculate the *platform sequence*.

A given sequence of products can be simulated with the timed Petri net model of the production cell. The figure below shows the Gantt chart of a simulated sequence. The marked gaps represent the set-up time. In this case the set-up time means the time when no product is inside the processing part of the production cell. The Gantt chart is built in Matlab 7.0.1 and it is one of the new features and functionalities of the Matlab Petri net toolbox [3].



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A QUEUE MODEL FOR THE OPERATIONAL PLANNING OF MARITIME CONTAINER TERMINALS

Angelo Alessandri[1] - Simona Sacone[2] - Silvia Siri[2]

[1] Institute of Intelligent Systems for Automation
ISSIA-CNR National Research Council of Italy
Via De Marini 6, 16149 Genova, Italy
email: angelo@ge.issia.cnr.it

[2] Department of Communications, Computer and Systems Science
University of Genova
Via Opera Pia 13, 16145 Genova, Italy
email: simona.sacone@unige.it, silvia.siri@unige.it

In the last decades, the number of maritime container terminals and the competition among them has increased considerably, therefore many research issues have arisen in that field. In particular, two overview papers concerning container terminal logistics ([2],[3]) describe and classify the main decision problems and optimization methods that regard logistics operations in container terminals.

The work proposed in this paper originates from the model for container terminals deeply described in [1], in which it is adopted at a strategic planning phase, in order to define some system parameters. Instead, here the same framework is applied in an operation planning phase, included in a simulation approach.

The model we propose is based on a set of queues; each queue represents a different container allocation stage in the area of the terminal, where containers are stored, depending on the transport modality and routing; the arrival/departure flows of containers by ships, trucks, and trains are suitably defined as stochastic processes.

The proposed model is then used in two different frameworks. At a planning level, the dynamic evolutions of the defined queues are described by discrete-time equations, where the state variables represent the queue lengths and the control variables regard the utilization of terminal resources as load/unload handling rates. Moreover, an optimization problem is defined, consisting in the minimization of the transfer delays of containers in the terminal; this cost function is in fact a performance measure of the overall terminal, specifically related to the queue occupancy. The problem is stated as an optimal control problem and it is faced according to a receding-horizon approach in which, at each time step, decisions are taken so as to minimize the cost function over a sliding horizon.

On the other hand, the same representation of the terminal by queues is adopted within a simulation context in which the system dynamics becomes event–oriented. The purpose of this framework is, of course, that of evaluating the system performance when adopting the results of the planning phase.

Moreover, the two frameworks designed and developed for the operation planning of the considered class of terminals can work in an integrated tool in which simulation and optimization coexist. More specifically, a simulation tool has been realized (and implemented by Arena 7.0), which represents the terminal dynamics when adopting a specific system configuration coming as a result of the optimization phase. A major feature of the designed simulation tool is, therefore, the possibility of pausing the simulation and running the optimization procedure which, on the basis of the system state, provides a possible new system configuration. This means that, in some particular instants, the simulation environment ”calls” the optimization model and this permits to change the configuration of some parameters or even some structural elements of the simulation model. Generally, this integration between the simulation and the optimization is quite significant since it allows to test the performance of the system and of the planning procedure even in case of disturbances or critical events requiring to re–configure the system.

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ASPECTS OF SIMULATION FOR PLANNING RAILWAY OPERATION

A. Schöbel, TU Vienna, Austria

Vienna University of Technology
Karlsplatz 13, 1040 Wien, Austria
Phone: + 43 1 58801-23211, Fax: + 43 1 58801- 23299
email: andreas.schoebel@tuwien.ac.at

Simulation is also used in planning railway operation because there is no possibility for testing timetables in real time operation. Moreover simulation is helpful in the planning process for dimensioning capacity of infrastructure. Another aspect for simulation is solving conflicts in real time operation because of delays of trains. Through the complexity of railway operation experienced users of simulation create often better solutions for practical application than theoretical methods.

Talking about simulation in the field of railway operation means a composition of dicrete and continous simulation in the class of dynamic simulation. An Example for the discrete aspect in railway operation is the timetable: trains start or end at a predefined date and time. The movement of these trains on a given infrastructure is a continous process. Another differentiation can be made in synchronous and asynchonous methods. Asynchonous methods are guided by a defined hierarchy of train categories, which was clearly defined in the past by a grade for each group of trains. New european legislation opens the market for new railway undertakings to sell time slots on the net of one infrastructure manager. So this requirement can easier be fulfilled by a synchronous simulation which uses a time-step-method.

So in this paper three aspects of the use of simulation in railway operation are described:

- Dimensioning of railway infrastructure
- Construction of conflict-free timetables
- Solving conflicts in realtime operation

In pratical use these aspects should not be considered as stand-alone problems because they have an effect on each other. The number of time slots for sale depends on the available infrastructure which has to constructed for a mix of different types of trains (persons, goods). So before constructing a new railway line planers should have an idea about how many time slots are needed for the market and what level of quality they need. In this early stage of planning the costs for the infrastructure are influenced. This also leeds to the comlexity of defining the capacity of a railway line which is depending on the timetable that has been appointed by several railway undertakings.

Todays state of the arte in the field of railway operation is characterised by the usage of simulation tools for planning of operation in different periods of a line – from construction and dimensioning until the solving of occuring conflicts. As a consequence of increasing use of software tools in railway operation, problems of data preparation, data administration and data exchange occurred. In the majority of cases tools were developed independently. Consequently tools from different companies are based on different data models and do not support integrative interfaces for data exchange.The data managment for these three scopes of railway simulation is getting easier through a standardised interface called railML. This is a scheme based on XML for the special issues of data exhcange on infrastructure, rolling stock and timetable. The organisation railML is an international, independent development partnership of railway companies and science organisations under the patronage of the Fraunhofer Institute Dresden for traffic- and infrastructure systems. A large field for development is the conflict defintion in a formal way related to the practical use. The solving process of conflicts cannot be described in a formal way because it is yet to complicated and also mainly based on the experiences of dispatchers. Moreover new european laws change the legislation of the conditions to define the sorts of conflict regarding to infrastructure manager and railway undertaking.

AN INTERNAL INTERNET TRAFFIC MODELLING/PERFORMANCE MEASURING TOOL

Jozef B. Lewoc, Leader (Leading Designer), Antoni Izworski and Slawomir Skowronski, (Wroclaw University of Technology)

Corresponding author: J. B. Lewoc
Leader (Leading Designer), ul. Powst. Śl. 193/28, 53-138 Wrocław, Poland
e-mail: leader@provider.pl

Extended abstract

In the early period of wide area network development, when researchers were widely employed in the network design teams, the problems of performance tests or rather measurements could be tackled rather easily. The detailed solutions applied in computer and communication networks were no secrets for the researchers. There were, also, no severe confidentiality-based limitation for publication of the results obtained. At present, the situation is quite opposite. The networking, especially connected with Internet, has been a profitable business for large-scale Public Telephone Operators (PTO's) for more than a decade. During that time, publications concerning Internet traffic modelling, traffic control and engineering, traffic measuring, testing results have become in a higher and higher degree some advertising studies.

In addition, even such description of the advertising character are very hardly available for internal traffic modelling, performance evaluation and testing tools. The reason is that such internal tools may be developed only in a close co-operation of researchers and network designers/operators. The big PTO's are no apt to let some external researchers to learn and, even more, to modify their detailed network solutions. Considering the fact of many apparent bugs (variable and often very long time needed for a message to reach the addressee, message delivery refusals and even lost messages in Internet) that tease many Internet users, they, most probably, do not employ their own researcher for such purposes, at least good ones. And if they do, the results obtained are rather unsatisfactory and very hardly available in the literature on networking, available in the public domain.

Some network researchers underestimate the basic difference between the internal and external tool, claiming that it is rather not important where the tool is to be implemented. This is some prove that many of them do not not know the network to be investigated because of the PTOs policy mentioned above. .

For the purposes of this paper, an internal measuring/testing tool is a program located in a TCP/IP network switch (node, router, gateway, etc.) and serving to generate artificial traffic and modelling/testing of network performance while an external one is a hardware and/or software system connected to the communication network and simulating a network subscriber or a group of subscribers, and serving similar purposes. Actually, most external testing/measuring tools are some realisations (models) of network subscribers and are limited to single subscriber interfaces. They can generate, therefore, only local Internet traffic. Of course, they may be very useful e.g. for the network protocol testing purposes. But in no way they can generate network traffic and measure performance on the overall scale of the communication network involved.

Considering the facts specified above, it seems to be worthwhile to propose the general structure and feasible functionality of an internal network performance testing/measuring tool intended especially for networks operating under the TCP/IP protocol suite. The proposal is based on the experience in development and applications of the internal network performance measuring tool Sitwa (from Polish System intensywnego testowania węzła = intensive node testing system).

Some results obtained with Sitwa are presented in order to show some possible benefits of an internal performance evaluation measuring tool . The results obtained cover the primary performance measures including round trip delay and and throughput in individual closed loops for some actual computer networks.

M/GX/1 QUEUING SYSTEM FOR THE MODELING OF REAL-TIME SERVICES OVER IP NETWORK

N. Kryvinska

Industry, Energy, and Environment WG, Department of Business Administration,
School of Business, Economics and Statistics, University of Vienna
Brünner Strasse, 1210 Wien, Austria
email: natalia.kryvinska@mail.austria.com

The queuing analysis is one of the most imperative tools for those involved with computer networking analysis. The number of questions that can be addressed with a queuing analysis is infinite and handles on virtually every area in computer and communication networks. The ability to make such an analysis is an essential tool for those involved in this field. Although the theory of queuing is mathematically complex, the application of queuing theory to the analysis of performance is, in many cases, remarkably simple. Knowledge of elementary statistical concepts (means and standard deviations) and a basic understanding of the applicability of queuing theory is all what is required. Equipped with these, the analyst can often make a queuing analysis on the back of an envelope using available queuing tables, or with the use of simple computer programs.

The modeling and analysis of system performance issues are useful tools in the development and engineering processes. The analytical models have a high value in the early stages to uncover major performance problems which affect the design of the architecture before the cost of rectification is too high. The development of new modeling methods for rapid analysis is very important for the fast deployment of new applications and services. And, after the examination of efforts done previously in this field (i.e., reference literature), we have discovered that there is a lack of studies in analyzing of network performance on 6, 7 levels of OSI (Open Systems Interconnection) model (e.g., presentation, and application/service level). It was a motivation to find mathematical models describing processes on these levels for the services support in IN (Intelligent Network) and IP networks. Therefore, in this paper, we develop a modeling method, based on queuing theory, for the solution of some problems faced when trying to support real-time services over IP. Namely, we are modeling signaling network architecture for the real-time services using M/GX/1 queuing system. We evaluate and compute expected waiting time and time in system. Furthermore, we present numerical results of our calculations and provide corresponding curves for them. In order to have precise values for time in system, we select and study M/GX/1 model. It supports more comprehensive formulas for waiting time and time in system than classic M/M/1 queuing model. The service and waiting time distribution for the IP real-time traffic differ from an exponential distribution (M/M/1 system). And, the M/GX/1 model is more relevant and adaptive to SIP server. In this model SIP server is assumed as a single server, with an infinite population of potential users, and users served in first-come-first-served order.

This paper is structured as follows. In sections 2 and 3, we introduce, motivate and design signaling network architecture using M/GX/1 queuing system. In the section 3, we perform mathematical analysis using queuing theory methods (e.g., queuing models behavior and performance in real-time systems, as well as evaluation of approximate formulas for the selected queuing models). Also, in the section 3, we present numerical results we have got from mathematical analysis. We give here strictly theoretical results in order to build stencil diagrams. Under “stencil diagrams”, we understand symbolic diagrams with purely theoretical values that can be used as stencils when practical results are gotten. To be precise, we give normalized values of main parameters (e.g., arrival rate, service time, time in system). And, when applying practical values of λ and μ, we have possibility to compare theoretical and practical results, that gives great opportunity to correct and adjust real, working system parameters for the better performance of whole network.

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Physical Modelling

MATHEMATICAL MODEL OF DYNAMIC HEAT TRANSFER IN A HUMAN-CLOTHING-ENVIRONMENT SYSTEM

Zhu Fanglong, Zhang Weiyuan and Liu Liying

Corresponding Author: Zhu Fanglong
Fashion Institute, Donghua University
No. 1882 Yan'an West Road, Shanghai city, China
Email: Pigzhu7979@mail.dhu.edu.cn

Clothing is an integral part of human life, and an understanding of the role of clothing in the thermal balance of the human body and thermal comfort under steady-state conditions has developed over the past few years [1-3]. The human body is rarely in a thermal steady state, but is continually exposed to transient conditions in physical activity and environmental conditions. Hygroscopic fibers such as wool and cotton absorb moisture vapor from ambient air when humidity rise, releasing heat. Similarly, when humidity falls, moisture is released and heat is taken up by the fibers. Under transient conditions, this sorption behavior of fibers plays an important role in the heat exchange between the human body and the environment, and in thermal comfort perceptions. In order to describe the transient heat transport behavior between body and environment, and to predict the dynamic thermal comfort of a "clothed man", we developed a mathematical model of heat transfer in microclimate in the paper. This model is solved by implicit finite difference method [4]. Such a model can be used to predict the temperature change in microclimate and to investigate the influence of dynamic heat transport behavior of clothing on the thermoregulatory process of the body. We also conducted a wear trial in a climate chamber under transient conditions, and we applied the predictions of the model to the results of the experimental investigations and compared the two. Predictions of the temperature at the inside surface of clothing agree well with the experimental results measured for garments made from wool and polyester fibers.

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047) ON THE NUMERICAL SOLUTION OF THE ONE-DIMENSIONAL SHALLOW SEA WAVES

A. G. Bratsos[1], A.M. Prospathopoulos[2] and I.Th. Famelis[1]

Corresponding Author: A.G. Bratsos, [1]Department of Mathematics,
Technological Educational Institution (T.E.I.) of Athens,
GR-112 10 Egaleo, Athens, Greece.
Phone: +30 210 5385308, Fax: +30 210 9630842
email: bratsos@teiath.gr
[2]Hellenic Centre for Marine Research (HCRM), Institute of Oceanography,
P.O. Box 712, GR-190 13 Anavyssos, Greece.

In this paper it is presented a parametric finite-difference scheme concerning the numerical solution of the one-dimensional Boussinesq-type set of equations, as they were introduced by Peregrine [4] in the case of waves relatively long with small amplitudes in water of varying depth. This set for the one-dimensional propagation using the assumptions of Beji and Battjes [1]) and Madsen et *al* [3] finally reads to

$$\frac{\partial \zeta}{\partial t} + \frac{\partial \left[(h+\zeta)\, u \right]}{\partial x} = 0,$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + g\frac{\partial \zeta}{\partial x} = \tilde{b}\, h^2\, \frac{\partial^3 u}{\partial x^2 \partial t} + h\, \frac{\partial h}{\partial x}\, \frac{\partial^2 u}{\partial x \partial t} + g\, b\, h^2\, \frac{\partial^3 \zeta}{\partial x^3}$$

in which $\tilde{b} = b + \frac{1}{3}$ and b the *calibration* factor.

The proposed method, which uses a parameter ϑ with $\vartheta \in [0, 1]$, can be considered as a generalization of the Crank-Nickolson method, aims to find the best values of the introduced parameter, which approaches in accuracy analogous methods known from the bibliography. The method has been applied successfully to the problem introduced by Beji and Battjes [1] ($\vartheta = 0.5$), as well as for other values of ϑ. The numerical results compared to the corresponding ones given by the MIKE 21 BW [2] developed by DHI Software, are encouraging and specific points for improvement and optimization of the method come out from the comparisons.

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On some convergence results and their relation to the impact of impurities on effective heat conduction properties

L. Flodén, A. Holmbom, M. Olsson and J. Silfver
Corresponding Author: A. Holmbom
Mid Sweden University
Campus Östersund, 83125 Östersund, Sweden
Phone: +46 63 165331, Fax: +46 63 165500
e-mail: anders.holmbom@miun.se

We consider a class of heterogeneous materials in terms of a sequence of heat conduction numbers $\{a^h\}$. For each h the temperature distribution evolves like the solution u^h to the equation

$$\begin{aligned} \partial_t u^h(x,t) - \nabla \cdot (a^h(x,t)\nabla u^h(x,t)) &= f(x,t) \text{ in } \Omega_T = \Omega \times (0,T)\,, \\ u^h(x,t) &= 0 \text{ on } \partial\Omega \times (0,T), \\ u^h(x,0) &= u_0(x) \text{ in } \Omega, \end{aligned}$$

where Ω is an open bounded set in $\mathbb{R}^N$. The sequence $\{a^h\}$ will contain different kinds of deviation from some mean including the possibilty of changing with time. Under certain assumptions on a^h the solutions u^h converges to the solution u to

$$\begin{aligned} \partial_t u(x,t) - \nabla \cdot (b(x,t)\nabla u(x,t)) &= f(x,t) \text{ in } \Omega_T, \\ u(x,t) &= 0 \text{ on } \partial\Omega \times (0,T), \\ u(x,0) &= u_0(x) \text{ in } \Omega \end{aligned}$$

for some b. This means that the effective properties of our sequence of materials stabilize near a material with heat conduction number b. For sufficiently strong convergence of $\{a^h\}$ the determination of b is immediate while a destabilization of this convergence makes this problem more difficult. The main complication from a mathematical point of view consists in the pairing of sequences of functions whose convergence are not strong enough to allow any immediate conclusions about what the limit looks like. We use certain multiscale techniques to investigate numerically and theoretically how much we can weaken the convergence of $\{a^h\}$ until the switch between these two situations appears.

SIMULATION OF HINDERED DIFFUSION IN SPATIALLY STRUCTURED DOMAINS USING A PARALLEL CELLULAR AUTOMATON

E. von Lieres and M. Finke, Research Centre Jülich, Germany
U. Buschmann, Siegen University, Germany

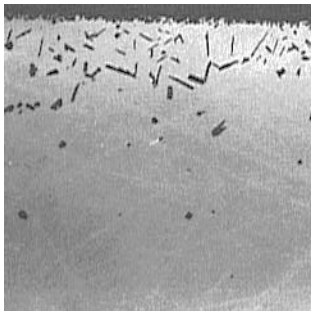
Corresponding Author: E. von Lieres,
Research Centre Jülich
Leo Brandt Strasse, 52425 Jülich, Germany
Phone: +49 2461 61-2168, Fax: + 49 2461 61-3870
email: e.von.lieres@fz-juelich.de

A parallel cellular automaton is implemented and applied for the analysis of hindered diffusion processes. The automaton is based on the three dimensional update rules of Chopard and Droz, where cubic cells are occupied by up to six diffusing particles. This automaton behaviour is realized by six basic cellular update patterns, namely ballistic trajectory, for symmetric deflexions and reflexion, which are chosen randomly, with different probability. The spatial structure of the domain is modelled by obstacles, which are implemented by inaccessible cells. Placement of these obstacles is based either on geometric rules or on measurement data. The cellular automaton is used to quantify the deceleration of diffusion processes resulting from different domain geometries. Hindered diffusion coefficients are estimated from the simulation results by comparison with analytical solutions of the differential equation for diffusion.

The cellular automaton is implemented in C++. System states are stored in octrees in order to reduce both computing time and memory consumption. The cell occupancy tree is traversed in each update step and discarded, after the updated occupancies are stored in a new tree. Unnecessary copying of obstacle, boundary and source cell positions is prevented by storing invariant information in separate octrees. A 64 bit architecture allows allocation of more than $2.000.000^3$ cells, whereas a 32 bit automaton is limited to 1.024^3 cells. However, both versions are maintained, since the 32 bit code performs better on certain machines. The automaton is parallelised using MPI by partitioning the domain into cuboids.

The cellular automaton is applied for studying, first, the migration of gas molecules in metal alloys with precipitates, which cause high temperature corrosion, and secondly, the transport of proteins in porous materials, which are used in liquid chromatography:

High temperature corrosion damages metal alloys which are exposed to gas atmospheres at high temperatures, for instance turbine rotors in power plants. A two dimensional cellular automaton was previously applied for the analysis of hindered gas diffusion in metal alloys with precipitates (see figure), because experimental observation of internal corrosion processes is difficult. This approach is now extended to three dimensions. At the same time, calculation times and memory consumption are significantly reduced by parallel implementation of the cellular automaton and octree based state storage.



Two dimensional cross section of a nickel base alloy with nitride precipitates

Mass transport in chromatographic media, which are used for protein separation, is predominantly diffusive and hindered by porous domain structure. Effective diffusion coefficients are, hence, important parameters for the rational design of stationary phases and purification schemes. Common methods for the quantification of hindered diffusion in chromatographic media analyse dynamic data from experimental observation of protein migration. In contrast, the cellular automaton approach utilises static data on matrix geometry and spatial hindrance structure, which allows studying the effect of arbitrary concentration profiles at the matrix boundary. From the simulation results, effective diffusion coefficients are estimated using a spherical diffusion model.

A LATTICE BOLTZMANN MODEL FOR PULSATIVE BLOOD FLOW IN ELASTIC VESSELS

D. Leitner[1], S. Wassertheurer[1], F. Breitenecker[2]

Corresponding Author: D. Leitner
[1] ARCS Seibersdorf Research GmbH, Div. Biomedical Engineering, A-2444 Seibersdorf
[2] TU Wien, Institut für Analysis und Scientific Computing, Wiedner Hauptstrasse 8-10, A-1040 Wien
email: dleitner@osiris.tuwien.ac.at

Abstract. Lattice Boltzmann Models (LBM) are widely used to solve fluid mechanical problems in engineering applications. For the cardiovascular domain we have extended this approach to support elastic walls as boundary conditions in order to simulate blood flow in elastic vessels. The flow is calculated in two spatial dimensions revealing characteristic flow patterns and geometrical changes of the arterial walls for different time dependent input contours of pressure and flow. The results of the model have been compared to the predictions of the model proposed in [1] which is based on the work of Womersley [2] and is widely used in blood flow simulation.

Introduction

In the western industrial countries cardiovascular diseases are the most frequent cause of death. Therefore a lot of research is done to get a better understanding of the cardiovascular system (CVS). To simulate the CVS various models of different accuracy are used and often coupled together to describe the circulation on different spatial and temporal scales. In this work two different approaches working on elastic vessels with diameters smaller than 5mm are compared. The first model uses the Womersley theory [1] [2]. The second model is a LBM. It simulates the blood flow in two spatial dimensions, solving the Navier-Stokes equation with the Lattice Bhatnagar-Gross-Krook (LBGK) method [3]. A new local rule for the elastic walls is introduced, which updates the position of the walls in every time step. Because the method works strictly locally it doesn't increase the complexity of the whole algorithm and enables a very efficient implementation . The results of the LBM are validated with the first model.

A Boundary Condition for Elastic Walls

The LBGK method can handle curved boundaries with different methods. In this work we have choosen the Fillipova-Hänel treatment that was examined in [4]. For the update rules of the walls we assume that the vessel is circular and deformation is axisymmetric and that the walls h are thin compared to the radius r, i.e $h/r \ll 1$ and tethered in the longitudinal direction. In this case we can use the circumferencel tensile stress τ_θ to establish a connection between transmural pressure p_e, Young Modulus E and radius r.

$$p_e(x) = \frac{4}{3}\frac{Eh}{r_0(x)}(1 - \frac{r_0(x)}{r(x,t)})$$

The transmural pressure $p_e(x) = p(x) - p_0$, where p_0 is the pressure of the surroundings, can be derived locally by measuring the pressure $p(x)$ in the lattice node next to the vessel wall, thus the wall can be updated locally in dependence of $r_0(x)$.

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A MODEL FOR HEAP BIOLEACHING OF CHALCOCITE WITH HEAT BALANCE: EFFECT OF GAS FLOW RATE

MARTIN J. LEAHY[a,b,*], MALCOLM R. DAVIDSON[a] and M. PHILIP SCHWARZ[b]
[a] Department of Chemical and Biomolecular Engineering, The University of Melbourne, Australia.
[b] Commonwealth Scientific and Industrial Research Organization, Division of Minerals, Australia.
[*] Corresponding Author, Commonwealth Scientific and Industrial Research Organization, Division of Minerals, Bayview Ave, Clayton, 3168, Victoria, Australia.
email: martin.leahy@csiro.au, ph. +61 03 95458500

Heap bioleaching is a hydrometallurgical process which can take place over a period of months to years, and chalcocite (Cu_2S) and pyrite (FeS_2) are often the minerals leached. Due to the low grade of the ore ($\sim 1\%$), the heaps need to be very large (up to a kilometer long, and typically less than 100m wide and 10m tall), to be economically viable. The heap bioleaching process involves the application of water based acid solution and the presence of bacteria (occurring either naturally or seeded in solution). To keep aerobic bacteria alive, air is injected (sparged) into the heap with pipes. The solution leaching the metal into solution, which is collected at the base of the heap for subsequent electrowinning processing. Leaching occurs as a result of ferric ions reacting with the sulfide minerals, producing ferrous and copper ions in solution, and resulting in the dissolution of pyrite. Ferrous ions are catalyzed to ferric ions in the presence of acidophilic bacteria such as *Acidithiobacillus ferrooxidans* and this increases the iron reaction rate by a factor of 10^4 compared to the direct chemical iron oxidation.

A discussion of gas flow rate reduction in heap bioleaching has limited coverage in the literature, with [4] providing the only modeling effort dealing with oxygen limitation where sparging has been taken into account. The present author also established the mechanisms under which gas flow rate reduction affects the heap leaching [3], with bottom up leaching the main result. However, the models mentioned do not consider heat generation and transfer in the heap; however, this may be a significant simplification since the heat produced and associated transfer was found to be extremely important in [2] and [1], with top down leaching found by [2].

In this work, we investigate the effect of gas flow rate reduction in a heap bioleaching model incorporating heat balance. The model also accounts for bacterial transport, attachment and detachment, and growth, and further biochemical and chemical reactions with ferrous and ferric ions, and pyrite and chalcocite in the ore. It is found that a reduction in the gas sparging rate improves the overall total copper extraction. Under a gas reduction, the heap initially leached from the bottom up due to initial oxygen limitation, before reverting to top down leaching with little oxygen limitation. The overall leaching in this case is better than under the full gas flow rate because the leaching in the (initial) upwards oxygen limitation leaching front is extensive, with the heap leaching under non-overheated conditions. Under full gas flow the heap becomes overheated quickly and little leaching occurs after this. Secondly, we find that further reduction in the gas flow rate causes periodic behavior in the important variables over time, due to oxygen, temperature and bacterial having coupled dynamics. The periodic behavior is fairly complex, with several variables interacting simultaneously. The cause of the periodic behavior is a result of the upwards oxygen limitation leaching front being retarded by the cool liquid advection under low ambient temperature from the top. A periodic process occurs when the upwards front is cooled and moves back downwards, before reestablishing and moving back upwards. During this periodic process, dependent variables such as the ferric concentration and rate of copper extraction rise and fall and accordingly.

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SHAPES OPTIMIZATION IN VISCOUS INCOMPRESSIBLE FLOWS BY SOLUTION OF THE INVERSE PROBLEM

N.B. Fedosenko

Center for Advanced Studies, Saint-Petersburg State Technical University
194251, Saint-Petersburg, Russia
fedosenko_n@mail.ru

In this work the method to obtaining the analytical solution of incompressible viscous flows is suggested. The results are used to investigating of inverse problem.

It is known, that the two dimensional non-steady equations of viscous incompressible flows are reduced to one equation of the fourth order concerning a stream function. The outcomes of the given work are obtained at direct usage of this equation.

The analytical solution of a boundary value problem for the Stokes is esteemed. As against the known solutions of infinite series, is suggested the solutions in a final form.

The main attention is given to statement of boundary conditions. The main difficulties arise in a three-dimensional case. By analogy with the introducing of a stream function, is approach with the introducing of a vectorial potential. In this approach the initial system will be converted to three equations at the component of a vectorial potential. Equations of a system it appears by bound only through boundary conditions (each speed depends on derivative a component of a vectorial potential on two directions.) It creates the main difficulties at closing of a boundary value problem. In the given work the path of solving these difficulties is suggested. The solutions are obtained not only in two dimensional, but also in a three-dimensional case are obtained.

The method of solution equations with the convective terms is offered. Thus the results obtained for the solution of equations of the Stokes will directly be used. For this purpose the special non-linear differential substitution of variables is offered. This differential substitution of variables sets a functional connection of the solution of a non-linear problem (with the convective terms) and solution of the conforming linear problem. The boundary value problem for the conforming linear equations is similar to a set of Stokes equations. The difference is, that the boundary conditions for linear (auxiliary) equations by a non-linear manner depend each on each. In this work the structure of relation of boundary conditions for (auxiliary) linear problem is offered. Then, by analogy with the solution of the Stokes problem, the analytical solution of this problem is obtained. After that with application of non-linear differential substitution of variables it is possible to obtain the solution of equations of incompressible viscose flows (with the convective terms).

For widespread results on cases with arbitrary domains the special analytical transformation of coordinates is suggested.

Modeling of a Two-axis Gimbal Test-Bed For Line-of-Sight Stabilization

K. Fadaei [1], M. Ataei [2] and S. Talebi [1]
Corresponding Author: K. Fadaei
1- Shahid Bahonar University of Kerman, Kerman, Iran
2- University of Isfahan, Isfahan, Iran
Phone: +98 9133320284
Email: kfadaei@gmail.com

Two degree of freedom seekers have many applications in aerospace and defense industries. The track sensor (i.e., TV camera, IR camera, laser, etc.) which is mounted on the inner axis of a two-axis mechanical gimbal detects the information reflects from the target in the sensor field of view (FOV). The track processor uses this information to generate rate commands that direct the gimbal bore-sight toward the target line-of-sight (LOS). LOS stabilization with the angular rate sensors mounted on the LOS axis is normally recommended for precision pointing applications [1]. This is accomplished by designing a control structure consisting of two servo loops; the outer tracking loop and the inner stabilization loop with appropriate bandwidths. The stabilization loop isolates the track sensor from platform motion, disturbances and external forces such as wind and air-stream inducing torque. The performance of this design depends on the understanding of the mechanical platform equations and also the accuracy of the mathematical model. In this paper, modeling of an available test-bed of a two-axis gimbaled seeker is considered. This is the first step along the final objective of stabilizer and tracker design and the controller is designed based on the resulted model. Therefore, modeling should be accomplished as accurate and complete as possible. For this reason, the equations present the system and also the mathematical relations between all variables in different parts should be derived. The test-bed under consideration consists of inner/outer gimbals, a tracking sensor, connecting push rods and cables, and two motors for inner and outer gimbals separately as shown in fig. 1. In order to model the test-bed in conjunction with an overall system concept the coupled two degree of freedom equations with cross products of inertia are used. The derivation of the equations in the case of no cross products of inertia was presented in [2]. The derivation of the equations of motion in the mass imbalance case was discussed in [3]. For the test-bed under consideration cross products of inertia are taken into consideration. The moments of inertia and also the cross products of inertia which are used in these equations are computed by mechanical simulator software.

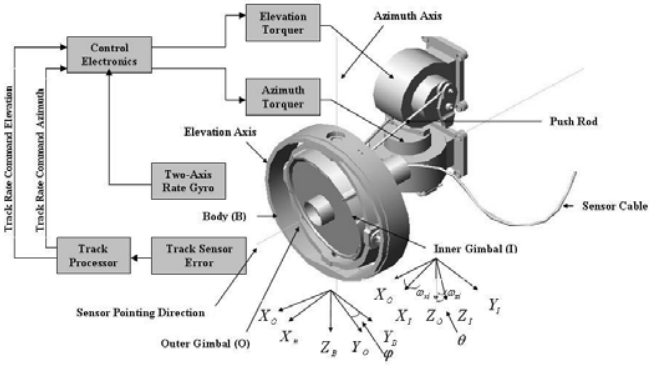

Fig. 1. Two-Axis Gimbaled Seeker Configuration

Since the developed torque by the motor is transferred to the gimbals through push rods, the related equations are derived and the dynamic equations of the system are modified by considering the relationships. In addition, the disturbances that affecting the pointing vector are modeled in two parts consisting base and coupling disturbances and then some comments regarding their attenuation and rejection are presented. Thus, an improved and more complete model of two-axis gimbaled test-bed under consideration is developed in such a way that consists the coupling term, cross products of inertia, linear and nonlinear friction and cable restraints, nonlinearity of the push rod and disturbance effects. Finally, this model is simulated and the simulation results are analyzed.

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OPTIMAL CONTROL OF QUANTUM SYSTEMS UNDER NON-MARKOVIAN CONSTRAINTS

W. Pötz, A. Goritschnig, and H. Jirari, University of Graz, Austria

Corresponding Author: W. Pötz
Institut für Physik, Theory Division
Karl-Franzens-Universität Graz, Universitätplatz 5, 8010 Graz, Austria
Phone: +43 316 3805228, Fax: +43 316 3809820
email: walter.poetz@uni-graz.at

In the recent past, there has been great interest in the study of the dynamics of elementary quantum systems. It has been prompted by the quest for implementation of quantum algorithms into actual physical systems.[1] Any realization of quantum information processing involves controllable unitary transformations (coherent steering) in form of coherent dynamics of the quantum system, preservation (trapping) of quantum states, as well as read and write operations. Control of a quantum system is rather limited when quantum interference between the dissipative process and the control are absent or neglected.[2] Although it is well known that the dynamics of a subsystem is inherently non–Markovian, in general, it appears from a study of the literature that optimum control with non–Markovian differential equations as constraints has not been studied to date in this context.[3, 4]

In this contribution we present indirect optimal control schemes for quantum systems which undergo non–Markovian dynamics. Dynamic control of a non-Markovian quantum system is formulated as an optimization problem in which the physical objective is contained in the cost functional and the system dynamics provides constraints in form of a set of non–Markovian and, in general, non-linear differential equations. Using the standard variational principle and, alternatively, the Hamilton-Pontryagin minimum principle, a general formulation of the optimality conditions is derived. As an application, the non-Markovian dynamics of a dissipative qubit represented by the spin-Boson model driven by an external field is discussed.[5] We present results for driving this spin 1/2 system (qubit) coupling to phonons along a prescribed trajectory $\rho_d(t)$ and trapping into a specified state ρ_T. Using both indirect and direct optimization schemes, it is shown that the coupling of the spin system to its bosonic environment can be controlled to a high degree provided that the system is addressed in the quantum regime.

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AIRFLOW-DEPENDENT MODELS FOR VIRTUAL SENSING OF THERMAL COMFORT

F. Felgner and L. Litz, TU Kaiserslautern, Germany

Corresponding Author: F. Felgner
University of Kaiserslautern
Erwin-Schrödinger-Straße 12, 67663 Kaiserslautern, Germany
Phone: +49 631 205-4208, Fax: +49 631 205-4462
email: felgner@eit.uni-kl.de

A fundamental problem in controlling thermal comfort is the measurement of all relevant quantities and the fact that they are, in general, dependent on space. According to the Predicted Mean Vote *PMV*, thermal comfort is determined by the temperature and the velocity of the air, the mean radiant temperature, the humidity and the respective person's clothing resistance and activity [1], [2]. Especially in air-conditioned rooms, thermal comfort can depend on the position within the room.
In a project supported by the German Research Foundation (DFG), a comprehensive strategy to control thermal comfort is being developed. Here, *PMV* will replace the punctiformly measured air temperature as control variable. A decisive point in this project is to conceive mathematical models describing the locally and timely varying air temperature $T_{\text{air}}(\vec{x}_i,t)$ and velocity $v_{\text{air}}(\vec{x}_i,t)$ at all positions $\vec{x}_i$ of current interest. These models will serve as virtual sensors substituting spatially distributed airflow and temperature sensors, which, in practice, could only be realized at unacceptably great expense. This contribution presents how such models can be made in a way they are fast enough to be applied online and, at the same time, accurate enough to evaluate thermal comfort at different positions in a room.
The typical way of modeling the airflow in a room is to use a highly resolved CFD model. The computing time of such a model is far beyond real time. A coarse mesh model that is suitable for real time use is usually too imprecise. Our approach is, therefore, not based on an online solution of the first principles but on a database of velocity and temperature results which are computed offline from a highly resolved CFD model. The database contains the behaviors of T_{air} and v_{air} for various air-conditioning scenarios. A scenario is characterized by a tuple $\underline{u}=(u_1,u_2,\ldots,u_n)$ of boundary conditions which are expected to influence the air temperature and velocity in those zones where persons are possibly located. For each scenario, the step response of T_{air} and v_{air} is recorded at various positions using the CFD simulator *Fluent*®. The simulation of the scenarios is automated by generating *Fluent*® command journals from the boundary condition space.
The online air model is given the actual boundary conditions and the position(s) under comfort observation. The model then approximates $T_{\text{air}}(\vec{x}_i,t)$ and $v_{\text{air}}(\vec{x}_i,t)$ by interpolating between the results of the nearest scenarios in the boundary condition space. This air model is integrated in a *Modelica* model of the room's walls which provides the mean radiant temperatures. By adding the measured humidity, a weather-dependent function for the clothing and the activity defined by the room's usage, $PMV(\vec{x}_i,t)$ is calculated (see figure).

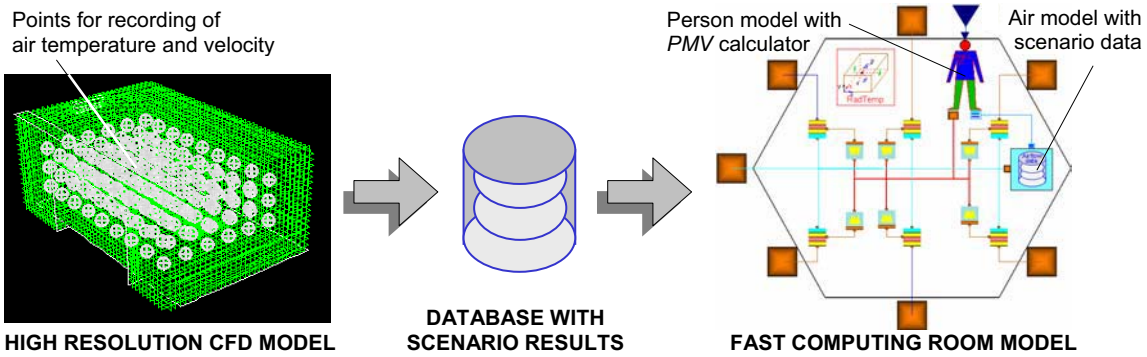

Figure: *Evolution of a model for the online estimation of thermal comfort*

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Education in Modelling and Simulation using ARGESIM Comparisons/Benchmarks with Physical Modelling

Florian Judex[1], Felix Breitenecker[1], Nikolas Popper[2]
[1]Vienna Univ. of Technology, [2]Drahtwarenhandlung – Simulation Services, Vienna; Austria

Corresponding Author:
Florian Judex, Inst. f. Analysis and Scientific Computing
Vienna University of Technology, Austria
Wiedner Hauptstrasse 8-10, 1040 Wien, Austria
Phone: +43 1 58801-11455, email: efelo@fsmat.at

ARGESIM started in 1990 the series *Comparison of Simulation Software* in the journal Simulation News Europe (SNE). These software comparisons developed towards benchmarks not only for simulation tools but also for modelling tools and for modelling techniques and modelling approaches.
The new comparisons C16 Restaurant Business Dynamics and C17 Spatial Dynamics of Epidemic, C18 Classical vs. Neural Net Models, and C19 Ground Water Flow address also non-classical modelling techniques, like agent-based simulation, neural nets and cellular automata. They can be analysed by various software systems, not only by simulation systems. Furthermore, they underline the importance of spatial dynamics, coupled with temporal dynamics. On the other side, classical comparisons with physical and mechanical modelling also allow for investigation by analytic methods.
The solutions allow comparisons of different modelling approaches, of features of simulators, of development of simulators, etc. Furthermore, the solutions – many of them with source codes – may be used as examples in simulation courses, etc.
The ARGESIM Comparisons have proven a big success: up to now 291 solutions have been published in SNE, and the comparison models are used worldwide as examples and benchmarks in teaching.

ARGESIM Comparisons as Education Tool. It has turned out, that the ARGESIM Comparisons are a valuable source for demos, exercises, or benchmark studies in education on modelling and simulation. As the comparisons tend towards modelling approaches, they can be used not only in simulation software classes, but also in more or less general classes on modelling in natural sciences, in computer science and computer engineering, etc.
Up to now, the model descriptions for all comparisons were given, as ODE, DAE, DEVS, or in another form. For education it is necessary, to study also the analytical modelling procedure, the derivation of the model, and the background of the laws which govern the model. Within a project for master theses and PhD theses, ARGESIM will extend the comparison definitions by information on modelling procedure, on the physical background, etc.
In order to make an ARGESIM comparison a self-contained part of a lecture, each comparison should consist of

i. Model description and derivation
ii. Application area and background
iii. Comparison definition
iv. Various solutions
v. Various implemented models (sources)

This contribution discusses the background of three physical – based comparisons and shows the possibilities for educational purposes:

- C1 Lithium-Cluster Dynamics, checks integration of stiff systems, parameter variation, and steady state calculation. Special problems are loops with logarithmic increments, correct double – logarithmic plots, steady state calculation; also approximations by Taylor series are possible
- C7 Constrained Pendulum, checks features for hybrid modelling, comparison of models, state events, and boundary value problems. Special problems are choice of states, different levels of hybrid approaches. Of educational interest is the fact, that the complexity of the model depends on the choice of state variables
- C12 Collision of Spheres, allows numerical or analytical analysis as well as continuous or discrete approaches. Interesting is a the broad variety of approaches (numerical - continuous, numerical – discrete, numerical – analytical, analytical – symbolic), and investigation of the convergence of collisions

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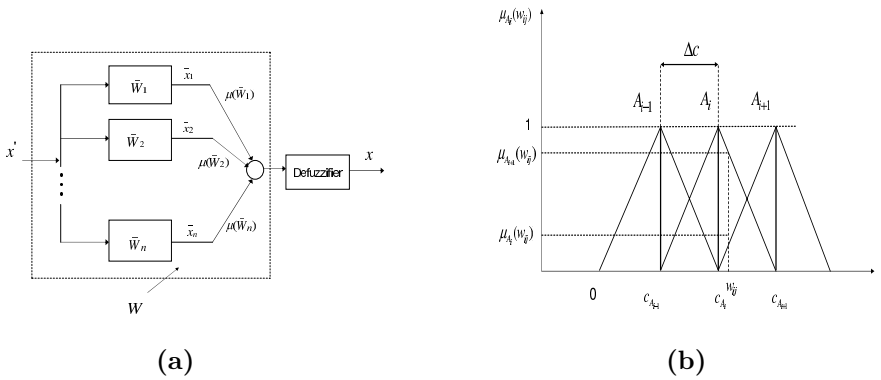
PATTERNS STORAGE AND RECALL IN QUANTUM ASSOCIATIVE MEMORIES

G.G. Rigatos [1] and S.G. Tzafestas

Unit of Industrial Automation
Industrial Systems Institute
26504 Rion Patras, Greece
email: grigat@isi.gr

Dept. of Electrical and Computer Eng.
National Tech. Univ. of Athens
15773 Zografou, Athens, Greece
email: tzafesta@softlab.ece.ntua.gr

Quantum associative memories are derived from the Hopfield memory model assuming that the elements of the weight matrix W are stochastic variables. The probability density function of the weights w_{ij} is calculated from the solution of Schrödinger's diffusion equation [1]. Indicative studies on neural structures based on quantum mechanics principles, can be found in [2-3].
Quantum associative memories demonstrate the particle-wave nature of information and are compatible with quantum mechanics postulates, such as: (i) existence in a superposition of weight matrices $\bar{W}_i$'s: it is shown that the weight matrix W can be decomposed into a superposition of matrices $\bar{W}_i$, thus increasing the number of stored patterns (attractors) by a factor of 2^N, (ii) evolution between $\bar{W}_i$'s with the use of unitary operators: it is proved that the evolution between the spaces which are spanned by the eigenvectors of the weight matrices $\bar{W}_i$ is performed through unitary rotations, (iii) retrieval of patterns that is analogous to a quantum measurement: it is shown that patterns recall is a random mapping described by the eigenvectors of the weight matrices $\bar{W}_i$.



(a) **(b)**

Figure 1: (a) Superposition of weight matrices $\bar{W}_i$'s (b) Strong fuzzy partition of weight w_{ij}

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[1]Corresponding author

MONTE CARLO METHOD FOR MODELING OF ELECTRON TRANSPORT IN QUANTUM WIRES

T. Gurov and E. Atanassov, IPP, Bulgarian Academy of Sciences, Sofia, Bulgaria
M. Nedjalkov and V. Palankovski, AMADEA Group, IuE, TU Vienna, Austria

Corresponding author: T. Gurov
IPP, Bulgarian Academy of Sciences
Acad. G. Bontchev Str., Bl. 25A, 1113 Sofia, Bulgaria
Phone: +359 2 979-6639, Fax: +359 2 870-7273
email: gurov@parallel.bas.bg

We consider a physical model of ultrafast evolution of an initial electron distribution in a quantum wire. The electron evolution is described by a quantum-kinetic equation accounting for the interaction with phonons. A Monte Carlo approach has been developed for solving the equation. GRID technologies are implemented due to the large computational efforts imposed by the quantum character of the model.

We consider a highly non-equilibrium electron distribution which propagates in a quantum semiconductor wire. The electrons, which can be initially injected or optically generated in the wire, begin to interact with three-dimensional phonons. We derive the equation, relevant for the evolution process, by a first principle approach in terms of the electron Wigner function. The evolution is quantum both, in the real space due to the confinements of the wire, and in the momentum space due to the early stage of the electron-phonon kinetics. The kinetics resembles the memory character of the (homogeneous) Levinson or Barker-Ferry models [1], but the evolution problem becomes inhomogeneous due to the spatial dependence of the initial condition. The latter is assumed with a Gaussian shape in both, energy and space coordinates. The obtained simulation results characterize the space and energy dependence of the evolution at zero temperature. Quantum effects introduced by the early time electron-phonon interaction are presented.

Monte Carlo (MC) methods are based on the simulation of stochastic processes whose expected values are equal to computationally interesting quantities. The random variable is said to be a MC estimator for the given functional if the mathematical expectation of the variable is equal to the functional. Therefore, we find an integral form of the quantum-kinetic equation and use the iterative expansion of the solution to construct a backward stochastic process. Then the desired physical quantities (values of the Wigner function, the energy and the density distributions) being functionals of the solution can be estimated simultaneously. Thus, by using common Markov chains for all these quantities, we achieve efficient implementation of our method.

We note the computational challenges posed by the equation. The kernel contains singularity,and the equation has a memory character. The variance of the MC estimator is bounded , but it depends exponentioally on the evolution time. Such behavior has been demonstrated also by stochastic approaches to Feynman path integrals [2]. We suggest an importance sampling technique which overcomes the singularity in the kernel. Since the variance depends on the evolution time, a lot of CPU power is needed for achieving acceptable accuracy at times above 100 femtoseconds. We divided the work into sub-tasks and submitted them to the EGEE [3] computational grid. Using a Resource Broker, the sub-tasks are distributed among EGEE sites (computer clusters). Results are collected and aggregated using an ad-hoc logging and bookkeeping system, which provides redundancy and fault tolerance.

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IDENTIFICATION OF TRANSPORT PARAMETERS FOR GALLIUM NITRIDE BASED SEMICONDUCTOR DEVICES

V. Palankovski and A. Marchlewski, AMADEA Group, IuE, TU Vienna, Austria
E. Ungersböck and S. Selberherr, Inst. for Microelectronics, TU Vienna, Austria

Corresponding author: V. Palankovski
TU Vienna, Gusshausstr. 27-29/E360, A-1040 Vienna, Austria
Phone: +43 1 58801-36017, Fax: +43 1 58801-36099
email: palankovski@iue.tuwien.ac.at

We present a methodology for the identification of transport parameters for Gallium Nitride (GaN) based semiconductor devices. A Monte Carlo (MC) approach has been employed to investigate carrier transport in GaN. Our model is validated against measured data and compared to published simulation results. It enables to understand effects taking place in this material system, and it provides inputs for macroscopic modeling of electronic devices. Material models which incorporate the basic characteristics of the carrier transport properties in a given semiconductor material are the physical core of device modeling. While for Silicon such models are well established, models for GaN and GaN-related materials are a hot topic of present research activities. This material system recently became of interest for applications in optical, high-power, and high-frequency electronics. Progress in assessing the entire material information is impeded experimentally by varying material quality and theoretically by the lack of detailed knowledge of relevant parameters. The MC method is a powerful technique to establish a consistent link between theory and experiments. We employ a single-particle MC technique to investigate stationary electron transport in GaN. Our model includes the three lowest valleys of the conduction band (Γ_1, U, Γ_3). Several stochastic mechanisms such as acoustic phonon, polar optical phonon, inter-valley phonon, ionized impurity scattering, and piezoelectric scattering are considered and their impact is assessed. The particular advantage of the MC method is that it provides a transport formulation on microscopic level, limited only by the extent to which the underlying physics of the system is included. Since the GaN material system is yet not so well explored, several important input parameters are still missing or just inaccurately known. As a particular example, Fig. 1 provides the electron drift velocity versus the electric field. We compare our MC result with other simulations, and with the very few available experimental data. The discrepancy in the MC results comes from different choices of parameter values and considerations of scattering mechanisms. Fig. 2 shows the low-field electron mobility in hexagonal GaN as a function of free carrier concentration. Our MC simulation is in good agreement with experimental data, although the scatter despite of similar measurement setup conditions is indeed pronounced. Note, that measurements of mobility over carrier concentration at low electric field are provided in the literature, but to the best of our knowledge no such MC simulation results have been published.

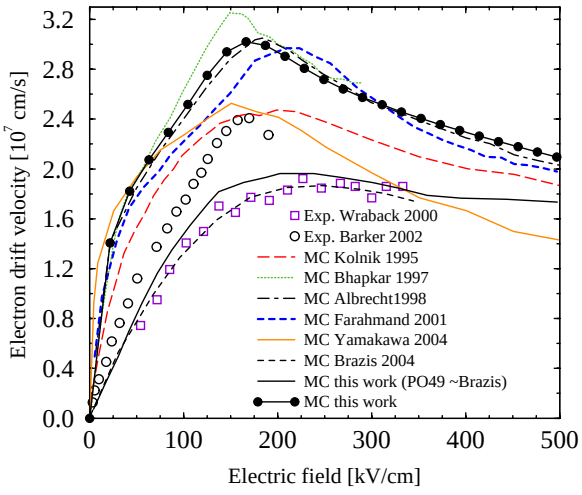

Figure 1: Electron drift velocity over electric field at carrier concentration of 10^{17} cm^{-3}.

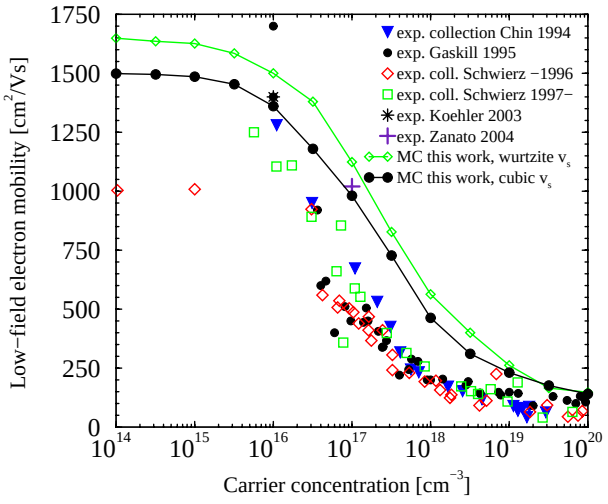

Figure 2: Low-field electron mobility in GaN as a function of the carrier concentration.

MULTI-SCALE BOND GRAPH MODEL OF THE ELECTROCHEMICAL DYNAMICS IN A FUEL CELL

A.A. Franco[a], P. Schott[a], C. Jallut[b] and B.M. Maschke[b]

[(a)] CEA-Grenoble/ Laboratoire de Pile à Combustible, France
[(b)] LAGEP, UMR 5007 CNRS/ Université Claude Bernard, France

Corresponding Author: A.A. Franco,
Commissariat à l'Energie Atomique (CEA) /DRT/DSEN/SGPAC/ Laboratoire de Pile à Combustible
17 rue des Martyrs, 38000 Grenoble, France
Phone: +33 4 38 78 63 75, Fax: +33 4 38 78 25 56
E-mails: alejandro.franco@cea.fr ; alesitofranco@yahoo.fr

Electrochemical impedance spectroscopy is a widely used experimental technique for the transient analysis of Polymer Electrolyte Fuel Cells. Experimental results are usually analyzed using equivalent circuit models which have to be fitted to each operation point and do not offer a direct access to internal physical parameters of the electrodes.

The goal of this paper is to present a novel multi-scale dynamic mechanistic Membrane-Electrode Assembly model [1] [2] [3] based on the distributed-parameter Bond Graph language [4] [5] [6] (irreversible thermodynamics and electrodynamics) and depending on the internal physical parameters. It is constituted of a transport phenomena description through the thickness of the electrodes and a physical description of the electrochemical interface between the Platinum and Nafion® phases at a nanoscopic scale.

We show how the bond graph language, extended to spatial multi-scale modelling, allows to structure this model in a modular way and to relate the multiple phenomena involved in fuel cell electrodes operation, like coupling between diffusion and migration of protons, and the electric potential dynamics.

Our model is mainly dedicated to the diagnostic of the dynamic fuel cell operation, and to help to define electrodes properties. Our approach allows to predict the influence of working conditions and operating point on the characteristics of the impedance spectra. The sensitivity of the simulations results to inputs like nominal current, temperature, reactant pressure and Nafion® and platinum loadings in the electrodes are in good agreement with experimental results [6].

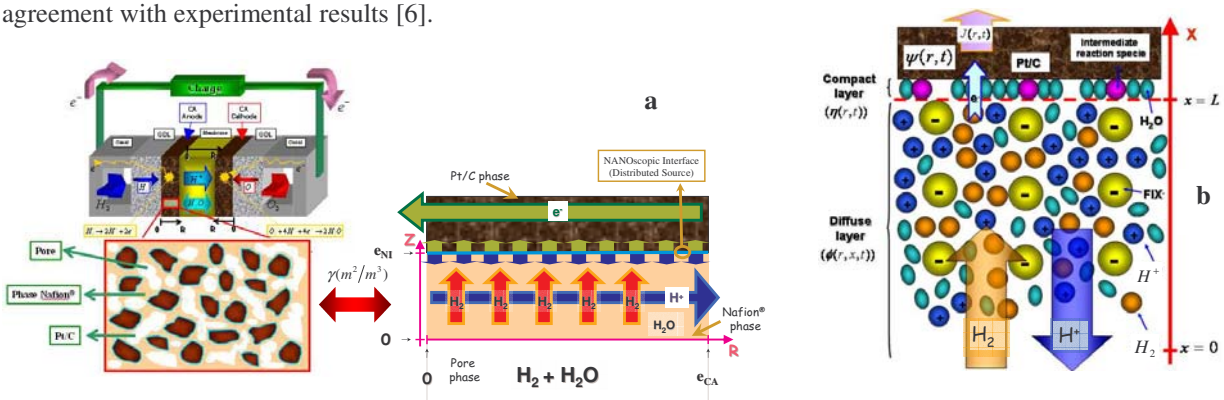

Fig. PEFC electrode morphology and the multi-scale model of the volumetric electrode (example of the anode) and localization (a) and detail of the nanoscopic interface model (b).

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DYNAMIC MODELLING AND SIMULATION OF A THREE-PHASE GRAVITY SEPARATOR

N. Al-Hatmi and M. Tham, University of Newcastle upon Tyne, UK

Corresponding Author: N. Al-Hatmi,
School of Chemical Engineering and Advanced Materials, Merz Court,
University of Newcastle upon Tyne. Newcastle upon Tyne, NE1 7RU, UK
Phone: 00447859053400, Fax: 00441912225292
email: N.M.al-Hatmi@newcastle.ac.uk

Three-phase gravity separators are one of the main surface production units in the petroleum industry. They are used to separate hydrocarbon streams produced at the wellhead into their constituent phases: gas, oil, and water, utilising the immiscibility and differences in the densities of the three phases. There are 2 categories: horizontal and vertical separators. Horizontal separators come in three typical designs, differing in the way the liquid levels are controlled: interface control with boot, interface control with weir, and bucket and weir. The most common is the configuration with interface control and weir. Although the separation mechanisms, sizing and design of such horizontal separators have been studied in detail, there are very few publications about their dynamics and control. This is surprising as efficient separator control is essential to the operation, safety and economics of oil production systems. An understanding of separator dynamics will enable the design of the suitable controllers needed to regulate gas pressure, water and oil levels. Thus, the aim of this paper is to develop a first principles dynamic model of a horizontal separator equipped with an interface control and weir, such as the one shown below.

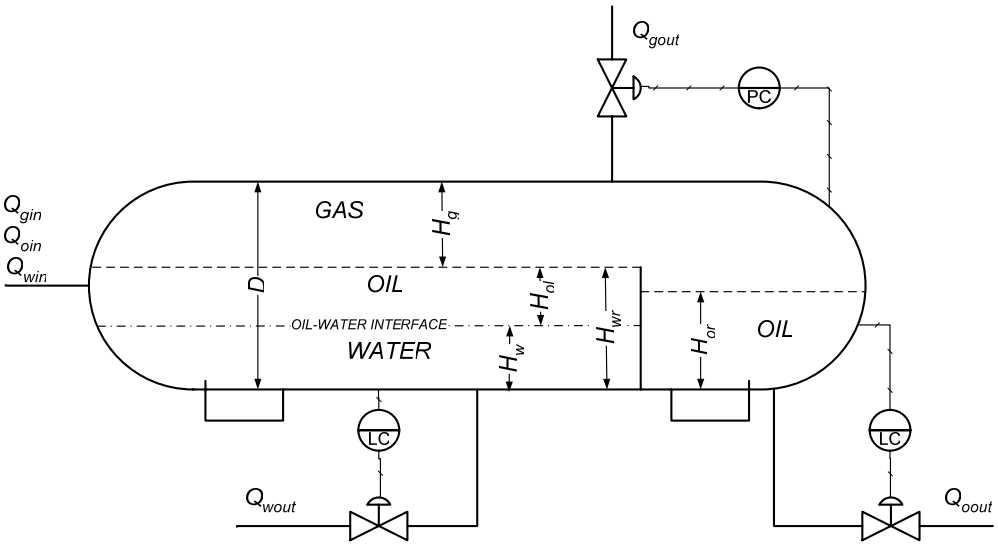

Figure 1: Schematic diagram of a gravity three-phase horizontal separator.

A number of assumptions were made when formulating the material balances: there is a complete separation between oil and water phases; the vapour phase behaves like an ideal gas and liquid densities are constant. In practice, separators are designed with internal fittings to promote laminar flow. In developing the model, the effects of such internals were assumed negligible. Nevertheless, the resulting set of equations is quite comprehensive and easily tailored to similar separators of different dimensions. The equations were solved using MATLAB-SIMULINK and the results revealed that the separator has an interesting mix of self-regulating and non-self regulating dynamics, giving insight into the behaviour of the separator especially when it is subject to slugs of gas in the feed.

Linear transfer functions between input and output variables were extracted by subjecting the first principles model to a series of step tests. These allow the degree of interaction between the variables to be quantified as well as controllability analyses to be performed, thus facilitating the design of linear control strategies – which is the next phase of work.

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Electrical and Power Systems

Noise Analysis of Phase Locked Loops using Stochastic Differential Equations

J. Anders and W. Mathis, University of Hannover, Germany

Corresponding Author: W. Mathis,
University of Hannover, Institute of Theoretical Electrical Engineering
Appelstrasse 9A, 30167 Hannover, Germany
Phone: +49 511 762-13595,
Fax: + 49 511 762-3204
email: mathis@tet.uni-hannover.de

The phase-locked loop (PLL) has become one of the most commonly used circuits in electrical engineering nowadays. Therefore, there is a great need for both a solid mathematical theory, especially in the presence of noise, and practical design rules that help the PLL designer to improve the circuit performance. Although numerous papers have been published on both issues separately, there is still a huge demand to make the, often times rather advanced, mathematical theory of stochastic differential equations, needed to accurately model the noise in PLLs, more accessible for the circuit designer with merely a basic background in stochastic calculus. This paper is intended to show that, thanks to the performance of modern personal computers, one can derive results with an accuracy comparable to the ones obtained from the so called Fokker-Planck technique using a Monte-Carlo simulation approach, that can be understood and used in practice with merely an average background in probability.

Since PLLs are widely used as the main component in receivers to synchronize a locally generated sinusoid with an incoming received carrier signal, our worked focussed on the accurate modeling of the PLL behavior in the presence of additive white Gaussian noise in the channel, that is the received signal is the original transmitted signal together with an additive delta correlated noise component with a Gaussian distribution. The corresponding block diagram, we have been using for our analysis is shown in Fig.(1) The main idea behind our approach was

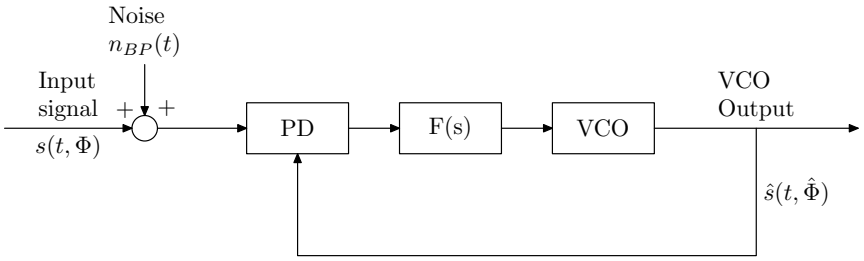

Figure 1: PLL configuration with bandpass noise process at the input

to take the existing numerical solution schemes for stochastic differential equations (SDEs), which had been developed throughout the past 15 years by Mathematicians like Kloeden and Platen (see [2]) and had already been successfully used in financial mathematics, to solve the SDEs describing stock volatility and apply them to solve the SDEs modeling the behavior of PLLs in the presence of noise. The main advantage of this approach lies in its simpleness, that is also the underlying theory is rather involved, applying the methods to a given problem can be accomplished by a design engineer with a basic background in the numerical solution of ordinary differential equations and some knowledge about random processes. The surprisingly high accuracy of this conceptually simple approach was shown by comparing our results with those obtained by Meyr and Ascheid (see [1]) using the Fokker-Planck technique.

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MODELING OF ELECTRICAL MULTIVIBRATORS BY SINGULARLY PERTURBED SYSTEMS

M. Prochaska, F.A. Probst, K. Bohle and W. Mathis, University of Hannover, Germany

Corresponding Author: M. Prochaska
University of Hannover, Institute of Theoretical Electrical Engineering
Appelstrasse 9A, 30167 Hannover, Germany
Phone: +49 511 762-13595, Fax: + 49 511 762-3204
email: prochaska@tet.uni-hannover.de

Since the beginning of the last century mathematical modelling of physical phenomena by means of relaxation oscillators became important. In the meantime relaxation oscillations play a decisive role for the modelling of chemical, physical and biological phenomena. In the field of electrical engineering relaxation oscillators provide a model for multivibrators. Since standard types are not able to produce high frequencies the so-called emitter-coupled multivibrator has replaced classical circuit concepts. In the last years emitter-coupled multivibrators received attention because of their suitability for high speed systems. Electrical multivibrators are important for the implementation of voltage controlled oscillators (VCO) in phase lock loop systems (PLL) which are key block in integrated transceiver circuits for mobile communication.

In this paper we present a nonlinear model of emitter-coupled multivibrators, where the parasitic components of the active elements are taken into account. Thus our model of the circuits can be simulated in contrast to previous publications. It will be shown that it possesses a high accuracy compared to circuit simulations with PSpice. The initial point of our analysis is the model of the multivibrator given by a regular singular perturbed system

$$\begin{aligned} \dot{\boldsymbol{y}} &= \boldsymbol{f}(\boldsymbol{y},\boldsymbol{z},\varepsilon) \\ \varepsilon\dot{\boldsymbol{z}} &= \boldsymbol{g}(\boldsymbol{y},\boldsymbol{z},\varepsilon) \end{aligned}, \tag{1}$$

where $\boldsymbol{y} \in \mathbb{R}^m$, $\boldsymbol{z} \in \mathbb{R}^l$ and m+l=n. By the theory of singularly perturbed systems a sub-model for the slow phenomena

$$\begin{aligned} \dot{\boldsymbol{y}} &= \boldsymbol{f}(\boldsymbol{y},\boldsymbol{z},\varepsilon) \\ 0 &= \boldsymbol{g}(\boldsymbol{y},\boldsymbol{z},\varepsilon) \end{aligned} \tag{2}$$

and with the stretched time variable τ a model for the fast motion

$$\begin{aligned} \frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}\tau} &= \boldsymbol{0} \\ \frac{\mathrm{d}\boldsymbol{z}}{\mathrm{d}\tau} &= \boldsymbol{g}(\boldsymbol{y},\boldsymbol{z}) \end{aligned} \tag{3}$$

is derived. Starting from these models we are able to analyze the slow and fast motion of the relaxation oscillation of emitter-coupled multivibrators in dependency on circuit components.

Since our model can be simulated, there are two significant advantages: First we are able to validate our results by means of the direct computation of the complete model. Second, we are able to analyze the slow as well as the fast phenomena. Especially the latter is in the field of emitter-coupled multivibrator a novel approach. So we are able to analyze the action during the transit time in detail. Moreover, detailed design recommendations can be derived: So we are able to reduce interfering oscillations to a minimum. Moreover, by means of our model the frequency can be calculated very exact. While typical approximations lead to errors of up to 40%, our numerical calculation, which is based on the nonlinear slow model, has an error of less than 3%. This big difference is caused by the piecewise-linear models which are common practice in the field of electrical engineering. Piecewise-linear modelizations are based on the estimation of the switching points of the transistors. The switching points of the transistors are associated with the bifurcation points on the slow manifold, which can be calculated by using a nonlinear model of the circuit. Of special interest is the result that the period time of the relaxation oscillation is proportional to the non-parasitic capacitance. In summery, our analysis shows the great value of mathematical methods in the field of nonlinear oscillations since the results can be used directly to achieve a better design of electrical circuits.

A NETWORK APPROACH TO THE MODELLING OF ACTIVE MAGNETIC BEARINGS

C. Collon, S. Eckhardt, J. Rudolph

Corresponding Author: C. Collon
Institut f. Regelungs- u. Steuerungstheorie
TU Dresden, D-01062 Dresden, Germany
email: Carsten.Collon2@mailbox.tu-dresden.de

The modelling of active magnetic bearings based on a network approach is considered. Using active magnetic bearings for the support of a rotating shaft yields contact free suspension as well as the possibility to position the shaft freely within the air gap. While stabilisation of the levitated shaft at a fixed position in the air gap can be achieved with linear methods based on linearised plant models, the design of controllers for trajectory tracking requires more evolved models of the plant. Exploiting the so called flatness property [3] of the process model, the design of nonlinear model based tracking controllers for tooling spindles in industrial manufacturing applications has been a field of intensive research of our group [2]. For the achievable overall system performance the quality of the models used to describe the magnetic bearings is of major importance and, hence, lies in the focus of the present contribution.

The force generated by a magnetic bearing is determined by the magnetic flux densities at the pole surface areas. Therefore, the key problem in modelling the force behaviour of a magnetic bearing is to describe the relation between the coil currents, the rotor position, and the generated flux density in the air gap. The spindle control has to be performed in real-time. As a consequence, a severe constraint on the complexity of the model is imposed by the available computational power. Network based modelling of active magnetic bearings provides an intuitive way to account for the position dependence in bearing models suitable for real-time control.

Describing and analysing technical processes of various physical domains with the help of networks is a well known and wide spread method. Regarding the analysis of magnetic fields deriving a network model with a reasonable number of network elements leads to a set of simplifying assumptions such as neglecting the stray flux or assuming a piecewise homogeneous field. Introducing a magnetic resistance leads to a lumped parameter description of the magnetic bearing. Carrying out a mesh flux analysis yields the describing network equations which are used to derive the position dependent current-force relation.

The modelling of a permanent magnet biased combined radial and axial bearing as introduced in [1] serves as an example to illustrate the application of the proposed approach. The results presented are based on measurements taken on a bearing provided by Levitec GmbH. For the centred shaft and moderate control currents a set of simplified linear networks is derived and the problem of parameter identification based on measured characteristic force curves is addressed. Due to the significant impact of saturation effects for higher control currents and eccentric shaft positions this bearing also serves as an example for showing how the integration of nonlinear network elements can improve the quality of the model without a significant increase of the computational effort required.

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ELIMINATION OF HOPF BIFURCATIONS WITHIN A POWER SYSTEM USING WASHOUT FILTER

I. Winzenick, Helmut-Schmidt-University, Hamburg, Germany*
M. Fette, System & Dynamik Beratungsunternehmen, Paderborn, Germany**
J. Horn, Helmut-Schmidt-University, Hamburg, Germany*
Corresponding Author: I. Winzenick

*Helmut-Schmidt-University, Hamburg
University of the Federal Armed Forces
Department of Electrical Engineering
Institute of Automatic Control Engineering
Holstenhofweg 85, 22043 Hamburg, Germany
Phone: +49 (0) 40-6541 3393
Fax: +49 (0) 40-6541 2822
email: Ingo.Winzenick@hsu-hh.de
email: Joachim.Horn@hsu-hh.de

**System & Dynamik
Beratungsunternehmen
Tempelhofer Straße 37
33100 Paderborn, Germany
Phone: +49 (0) 5251-40404
Fax: +49 (0) 5251-40406
email: fette@systemdynamik.de

An electric power system is one of the most complex systems and highly nonlinear. Growing ecological pressure as well as political reasons result in an increased demand on renewable energy sources, which have to be implemented. Furthermore off shore wind farms have to be installed in addition to new technologies like fuel cells. The economical necessity to achieve more trading options causes new needs in strategies to control the power flow adequately. Therefore e.g. flexible AC transmission systems (FACTS) are used.

All these influences change the dynamic behaviour of the system qualitatively. Based on economical analysis the power industry is interested in reducing of their overcapacities in order to increase their competitiveness. Because of this and the increasing demand for electric energy the system will be driven closer to its physical limits. So, nonlinear effects become more dominant. Nonlinear oscillations can already be detected. Furthermore Hopf bifurcations can be related to such incidents. A bifurcation point (or short bifurcation) represents a characteristic point of the system, where it changes its behaviour qualitatively if a parameter (e.g. the load demand) is changed. A rather simple introduction of the Hopf bifurcation will be given within the paper. Further information can be found in literature which is referenced in the paper.

A known possibility to create and influence Hopf bifurcations by using washout filter aided nonlinear control functions is used and briefly presented. The results are adopted to power systems although Hopf bifurcations are usually unwanted. Therefore a well known power system model will be chosen and equipped with such a control law to show the effect of the washout filter aided control law on the system.

At first the design of the washout filter is shown by using a rather simple dynamic system. Then the method is adopted to characteristic power system models. These models -especially the bifurcational behaviour- are analyzed with and without the control law in order to present the effect on desired dynamical properties of the system and their major dependencies.

A strategy to determine the gain intervals of the washout filter aided control law is presented and stable operation areas can be identified. Within this interval, Hopf bifurcations are in principle 'eliminated' or 'moved' to enlarge the stable operation area which is illustrated by adequate bifurcation diagrams. The presented curves are calculated by using continuation methods. Combined with sophisticated test procedures paths of critical points (e.g. Hopf bifurcations curves) can be tracked. The paper summarizes the results and gives an outlook on further applications on power system controller design.

SIMULATION OF POWER OSCILLATIONS AND PRESSURE PULSATIONS IN A HYDRAULIC SYSTEM INDUCED BY CAVITATING VORTEX ROPE

Corresponding Author: Dr.-Ing. Jiri Koutnik

Voith Siemens Hydro Power Generation
Alexanderstraße 11, 89510 Heidenheim, Germany
Phone: +49 7321 37 2631, Fax: +49 7321 37 7037
email: jiri.koutnik@VS-Hydro.com

1. Introduction

At Francis turbines operating at higher loads then the optimum one (Full-load) a cavitating vortex rope below the runner outlet is formed because of the swirl flow and the corresponding pressure distribution. Such a cavitating rope may under certain condition act as an energy source, which leads to self-excited pressure oscillations in the whole hydraulic system.

These pressure oscillations induce consequently turbine power oscillations, which may reach unacceptably high values.

2. Methods of simulation

There are two possible ways how to simulate the above described phenomenon:

a) Modal analysis of a linearized model of the hydraulic system including a special model for the cavitating vortex rope
b) Nonlinear simulation of the complete system in the time domain (hydraulic system, turbine, generator, turbine controller, rigid grid)

The modal analyses is carried out using a software based on the Transfer Matrix Method with hyperbolical functions [1]. Individual pipe elements are described with partial differential equations with status variable of pressure and discharge. The observed system physical behaviour is typical for an unstable system, therefore its complex natural values are analysed. With such a procedure can be determined the stability limit and prediction of the frequency only. An example of such analysis will be shown and compared with measurement results.

The non-linear analysis allows quantitative prediction of the pressure and output amplitudes. For the generator model the 2 axis Park-theory is used [2]. Example of such a simulation will be shown as well, and comparison with measured time signal presented.

3. Summary

The presented comparison of calculated and measured results shows qualitative as well as quantitative agreement and thus the theory used is confirmed.

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THE MODELLING OF THE GHAZI-BAROTHA HYDRO-POWERPLANT FOR THE PURPOSE OF THE TRAINING SIMULATOR

S. Blažič, D. Matko, University of Ljubljana, M. Letonje, M. Clemente, Iskra sistemi, d.d.,
I. Škrjanc, University of Ljubljana, Slovenia

Corresponding Author: S. Blažič
University of Ljubljana, Faculty of Electrical Engineering
Tržaška 25, SI-1000 Ljubljana, Slovenia
Phone: +386 1 4768763, Fax: +386 1 4264631
email: saso.blazic@fe.uni-lj.si

This paper presents the design of the simulator for the hydro-powerplant (HPP) Ghazi-Barotha. The latter is located in Pakistan in the upper flow of the Indus river, approximately 100 km to the south of Islamabad. The HPP consists of the barrage, the power channel (its length is 51.9 km, nominal flux is 1600 m^3/s, and the water depth is 9 m), and the power complex. The main parts of the latter are 5 generators (cumulative power is 1450 MW) and a 500 kV high-voltage switchyard (6 bays connecting 6 power lines).

From the figures above it can be seen that the HPP is a huge object. An extensive control and supervisory system has been built that is used for changing modes of operation, starting up and shutting down the HPP and many others operations. In spite of that, the human operators are present all the time and can react in the case of difficulties. It is also possible to run the HPP in manual mode. For these reasons, the operators have to be very familiar with the plant and the consequences of all their actions. To achieve this level of knowledge, all operators have to undergo a special training to be capable of solving different problems they may encounter. The HPP is neither suitable nor acceptable for the training, and therefore one of the demands of the contractor was that a special training simulator has to be built.

Before building the simulator, a deterministic model of the plant has to be available. This paper focuses on the modelling issues involved in this process. Since our model is used for training purposes, it does not have to be very precise but it has to show similar qualitative behaviour as a real plant. For that reason, unimportant components of the system are not modelled. This is quite important if we have in mind that tens thousands of binary signals and several thousands of analogous signals are actually measured on the plant.

The paper is focused on the hydrodynamic model of the plant. The most interesting subsystem from the theoretical point of view is the power channel. At first, it was modelled as a distributed system, and then the lumped parameter approximation was obtained to model the dependencies between the fluxes and the water levels at the channel inlet and outlet, respectively. The inputs of this submodel are therefore flux at the inlet and the one at the outlet, while the outputs are upstream and downstream water-levels. This approach had to be taken to make use of the data that were available for the gates (dependence between the upstream water level, downstream water level, and the flow). The problem of the impedance channel model is that the operating point is poorly defined. This is overcome by a non-classical approach in the system, namely a combination of admittance and hybrid model was used to model the channel. The “hydrodynamic” model is completed by adding the models of the standard gates, undersluice gates, head regulator gates, tail regulator gates, and pond models. Those models were obtained using the data provided by the designers of the gates. The main difficulty here was the lack of data in some operating conditions which was partially solved by including some heuristic knowledge. In spite the fact that the plant is quite complex and several components were poorly known, the simulator results of the hydrodynamic model are almost exactly the same as the response of the actual system.

The “electrical” part includes the model of five turbines and corresponding units and the model of the high-voltage switchyard. This model is much more extensive than the “hydrodynamic” part, but on the other hand the underlying models were drastically simplified, i.e. the “electrical” part of the plant was modelled as a static system since its dynamics are very fast compared to the dynamics of the “hydrodynamic” part. Slight exception of this rule is the simulation of the starting procedure of the turbine that was modelled as an automaton, i.e. the next phase in the procedure starts after the completion of the previous one.

The whole model of the HPP was realised as a discrete time system and implemented in the executable designed in C++ and run in the Windows environment. The computer implementation of the simulator brought several programming and communication issues not analysed in this paper.

COMPUTER MODELING AND SIMULATION OF ELECTRICAL POWER SYSTEMS

Giuseppe Fusco and Mario Russo, University of Cassino, Italy

Corresponding Author: G. Fusco
Università degli Studi di Cassino
Via G. Di Biasio 43, 03043 Cassino (FR), Italy
Phone: +39 0776-2993688, Fax: +39 0776-2993707
E-mail: fusco@unicas.it

The use of computer simulations is of great importance when dealing with electrical power systems which represent large scale systems composed of complicated and sophisticated combination of multiple electronic and electromechanical components. In general, these components are nonlinear. Dynamic studies of power system under normal operating conditions require the writing of a system with an huge number of equations. By the way, it is easy to understand that embedding all the dynamics affecting the power system in a comprehensive analytical model of the overall plant does not lead to a tractable performance analysis tool. For this reason, in these studies, usually just a small portion of power system is modeled in detail and the rest of the system is represented by simple equivalent circuits. From this point of view, the availability of a computer model leads to setting up simulation tests that represent both a low-cost, safe and fast performance analysis tool and a computer-aided design tool of the control scheme. Furthermore, a modular arrangement of the computer model simplifies the representation of the complex dynamical power system, while letting readable the nature and the role of each module to the whole dynamics. The paper describes a general purpose modular computer model for the simulation of a power system suitable for conducting analysis and control studies. It comprises all the main components present in a large power system: namely generating units, transformers, transmission lines, electronic actuators, transducers and loads. Such components are accurately modeled and simulated in the time-domain. The computer model also takes into account the presence of measurement noise and saturation of the signals. In particular, the generating units are modeled with the synchronous generator including excitation system, power system stabilizer and turbine/governor dynamics [2, 3]. The availability of a simulation package also enables to identify the structure and parameters of an approximated discrete-time linear model describing the power system dynamics from a given bus and for an assigned operating point. The model that is analized refers to a nodal voltage amplitude and to a voltage control device. Starting from input/output data collected during simulation study, the polynomial orders and parameters of a such model are estimated by resorting to the use of classical Least-Squares (LS) technique to calculate the residual prediction errors [1]. Eventually, the proposed computer models have been applied to simulate the operation of a three-phase 220 kV - 50 Hz power system. Using the simulation results, the LS algorithm has been used to estimate an approximated discrete-time linear model of the system with reference to a FC-TCR Static VAr System connected at a chosen busbar. The estimation has been performed and compared for different model structure. Finally, the step response of one of the estimated models is simulated and compared with the step response of the actual power system.

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A NUMERICAL SIMULATION OF THE DYNAMIC BEHAVIOUR OF A DIRECTLY WOOD PARTICLE FIRED GAS TURBINE

F. Wingelhofer and B. Glöckl, Vienna University of Technology, Austria

Corresponding Author: F. Wingelhofer
Institute of Thermodynamics and Energy Conversion
Vienna University of Technology
Getreidemarkt 9 / 302, 1060 Wien, Austria
Phone: + 43 1 58801-31314, Fax: + 43 1 58801-31399
Email: Franz.Wingelhofer@TUWien.ac.at

Compared with the combustion of gaseous or liquid fuels, the combustion of solid fuels like wood particles takes much more time. This fact leads to a larger combustion chamber if wood fuel is supposed to be directly fired in a gas turbine, originally designed for firing gaseous or liquid fuels. As wood fuels contain in general also some portions of ash, an ash separation of the hot gases upstream of the turbine is required for a safe operation. Both, the large combustion chamber and the device for ash separation result in a large volume between the compressor and the turbine. Due to high pressure and high temperature of the gases in this large volume, a high amount of energy is stored.

During regular operation of the gas turbine, the storage of energy in the combustion chamber and the device for ash separation lead to a slower response on load changes. Since a directly wood particle fired gas turbine is not designed to operate detached from the main grid, the storage of energy is not a real problem. But the storage of energy can become a severe problem if the generator of the gas turbine gets detached from the main grid instantly. At the first moment, the gas turbine rotor is not retarded by the generator any more, leading to an increasing speed of the gas turbine rotor. Depending on the load right before the detachment as well as on the amount of energy stored in the combustion chamber and the device for ash separation, a high overspeed of the gas turbine rotor will occur. An overspeed control has to take care for an opportune reduction of the fuel mass flow.

In this paper, a transient model for a numerical simulation of the dynamic behaviour of the directly wood particle fired gas turbine, as installed in the laboratory of the Institute of Thermodynamics and Energy Conversion, is presented. Figure 1 gives a schematic overview on the gas turbine plant. Special features of the directly wood particle fired gas turbine are the usage of a commercial gas turbine designed for oil firing, a pneumatic fuel feeding system, a two stage combustion chamber and an axial cyclone as device for ash separation of the hot gases upstream of the turbine. In the primary stage of the combustion chamber wood fuel gets gasified autothermally, producing a low calorical gas which is burned in the secondary stage completely.

Since the gas turbine behaviour owing to a detachment from the main grid is a very critical factor for a safe operation, the numerical simulation concerns mainly with the detachment from the main grid. The mathematical model used for the numerical simulation with MATLAB/Simulink is presented in detail. Three different overspeed control devices are discussed and investigated whether they are able to limit the speed of the gas turbine rotor and to enable a safe operation of the directly wood particle fired gas turbine plant. Further, the paper includes a detailed discussion of the obtained results.

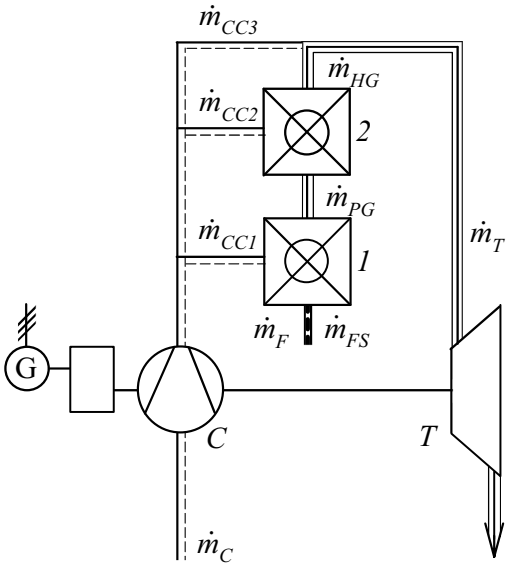

Figure 1: Directly wood particle fired gas turbine as installed in the laboratory of the Institute.

CAUSAL CHANNEL INVERSION FOR MIMO ISI SYSTEMS: EQUALIZATION ERROR MODELING AND ROBUSTNESS

Nikola Vucic
Fraunhofer German-Sino
Lab for Mobile Communications MCI
Einsteinufer 37, 10587 Berlin, Germany
nikola.vucic@hhi.fhg.de

Holger Boche
Technical University Berlin
Heinrich Hertz Chair for Mobile Communications
Einsteinufer 25, 10587 Berlin, Germany
holger.boche@mk.tu-berlin.de

The problem of constructing the channel pseudoinverse in a frequency selective, multiple-input multiple-output scenario becomes intricate if causality and robustness constraints are imposed. In this paper, the receive filters of interest will be the ones that either minimize the noise enhancement, or improve robustness, under a certain limit on the equalization error with respect to the perfect channel inversion.

The analog expression for the Moore-Penrose pseudoniverse in the frequency selective case is given as $\boldsymbol{H}(z)^{\ddagger} = \left(\boldsymbol{H}(z)^{*}\boldsymbol{H}(z)\right)^{-1}\boldsymbol{H}(z)^{*}$ [1]. It can be easily noticed that this expression renders in general an IIR filter which is non-causal and non-realizable in practice. In [2], it has been shown using the theory of Banach algebras that a causal left inverse of $\boldsymbol{H}(z)$ exists if and only if

$$(\exists \delta \in \mathbb{R}) \quad \boldsymbol{H}(z)^{*}\boldsymbol{H}(z) \succeq \delta^{2}\boldsymbol{I}, \quad \forall |z| > 1. \tag{1}$$

However, the analytical closed-form solutions for the construction of the practically realizable causal left inverses seem intractable.

In order to explain robustness modeling, assume that the channel is estimated erroneously at the receiver with $\boldsymbol{H}(z) = \boldsymbol{H}_{C}(z) + \boldsymbol{\Delta H}(z)$, where $\boldsymbol{H}_{C}(z)$ is the exact channel and $\boldsymbol{\Delta H}(z)$ is the estimation error, characterized with its energy norm constraint $\|\boldsymbol{\Delta H}\|_{E} \leq \mu$. It is proved that the equalization error is tightly upper-bounded with $\mu\|\boldsymbol{G}\|_{E}$ in this case, which clarifies the desire for controlling the filter energy norm.

Based on the previous work [1, 2], it is known that the ideal, non-causal pseudoinverse is the left inverse with the minimum H_2 norm (the measure of the noise enhancement) and the minimum energy norm $\|\boldsymbol{H}^{\ddagger}\|_{E} = \delta^{-1}$, where δ is the largest constant so that (1) is valid, and which is independent of system dimensions. Interestingly, these characteristics do not fully extend to the case when causality constraint is imposed, and the energy norm control of any non-symmetric practically realizable pseudoinverse seems difficult. Their minimum energy norm does not only depend on the constant δ from (1), but also explicitly on the number of inputs in the system [1, 2].

The intractability of the closed form solutions for practically realizable and possibly robust pseudoinverses motivates the search for a numerical framework which will be able to handle constraints based on the filter H_2 and the energy norm. In this direction, the concept of upper-bounded norms is employed for modeling the equalization errors, in order to support cases when no exact inverse exists. The problems of equalization filter construction with the goals of minimizing the noise enhancement or improving the robustness under the imposed error constraints are proved to be equivalent to the standard semidefinite programming problems, which enables the application of efficient numerical methods. The focus is put on channels and filters with FIR. However, some discussions of the IIR case are given, as well. The full system simulations are performed for random MIMO-ISI channels.

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The Peak-to-Average Power Reduction Problem–Fundamental Limits and Connection with Fourier Analysis

Holger Boche and Volker Pohl, TU Berlin

Corresponding Author: Holger Boche
Technical University of Berlin, Heinrich-Hertz-Chair for Mobile Communications
Einsteinufer 25, 10587 Berlin, Germany
holger.boche@mk.tu-berlin.de

A major problem in multicarrier communication systems such as orthogonal frequence-division multiplexing (OFDM) is the unfavorable crest-factor, i.e., the square root of the peak-to-average power ratio (PAPR) of the transmit signal [1]-[3]. Various algorithms have been developed to tackle this problem. For some further motivation, literature and related results see [4]-[6].

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Modelling of Distributed-parameter Systems for Control Purposes

MODEL INVERSION FOR DISTRIBUTED–PARAMETER SYSTEMS USING SUMMABILITY METHODS

T. Meurer and M. Zeitz, Univ. Saarland and Univ. Stuttgart, Germany

Corresponding Author: Thomas Meurer
Chair of System Theory and Automatic Control, Saarland University
P.O. box 151150, 66041 Saarbrücken, Germany
Phone: +49(0)681 302-64724, Fax: +49(0)681 302-64722
email: thomas.meurer@lsr.uni-saarland.de

Rigorous process modeling leads to a distributed–parameter description in terms of partial differential equations (PDEs), whenever spatial or dispersed–phase effects have to be taken into account. Common examples include flexible structures in mechanics as well as diffusion–convection–reaction systems in chemical engineering. For these systems, typically complex dynamical behavior evolves, which complicates analysis and control design.
From a control perspective, it can be observed that model–based control design methods for distributed–parameter systems (DPSs) are mainly directed towards the solution of the stabilization problem [2], while only few analytical approaches exist for the design of tracking control for DPSs, e.g. to realize high–performance positioning tasks in robotics or set–point changes during startup, operation, and shutdown of fixed–bed tubular reactors. However, the recent extensions of flatness–based methods to the distributed–parameter case (see e.g. [6] and the references therein) have provided new possibilities to solve tracking control problems for DPSs. Thereby, feedforward tracking control is systematically determined based on the inversion of a given plant model as schematically outlined in Fig. 1: the input trajectory $u^*(t)$, which is needed to track a desired trajectory $y^*(t)$ prescribed suitably from the signal generator Σ^*, is obtained from the inverse model Σ_∞^{-1} of the DPS Σ_∞.

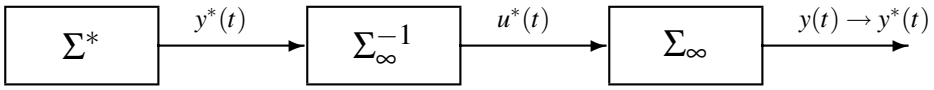

Fig. 1. Inversion-based feedforward control for DPS Σ_∞ with inverse model Σ_∞^{-1} and signal generator Σ^*.

Obviously, the determination of Σ_∞^{-1} requires the inversion of the infinite–dimensional model Σ_∞. For a certain class of parabolic DPSs with boundary input, the inversion can be obtained using formal power series (FPS) [4]. Thereby, system states and inputs are parameterized in terms of a parameterizing function and its time–derivatives up to infinite order. The applicability of the formal solution is rather limited due to the required proof of uniform series convergence, which is related to the problem of trajectory planning [6].
In this contribution, summability methods [1, 3] to sum slowly converging as well as certain divergent series are considered to extend the range of applicability of FPS and to solve the model inversion problem [5]. Therefore based on a simplified model of a tubular reactor in terms of a single nonlinear parabolic PDE, model inversion using formal power series is exemplarily studied with the focus on the application of summability techniques for enhanced trajectory planning. It is thereby shown that k–summation [1] and its proposed variant the so–called (N,ξ)–approximate k–summation [5] provide powerful summation approaches in view of the solution of the feedforward tracking control problem for distributed–parameter systems. This is confirmed by simulation results for the tubular reactor model at different stages of operation, which illustrate the broad range of applicability of the considered approach.

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HYBRID MODELING OF A STRATIFIED STORAGE TANK

T. Kreuzinger*,[1], M. Bitzer*, Robert Bosch GmbH, Germany
and W. Marquardt**, RWTH Aachen, Germany

*Mechatronic Engineering
Corporate Sector Research and Advance Engineering of Robert Bosch GmbH
Robert–Bosch–Strasse 2, 71701 Schwieberdingen, Germany
Phone: +49 711 811 – 1228
email: {tobias.kreuzinger,matthias.bitzer2}@de.bosch.com

**Lehrstuhl für Prozesstechnik, RWTH Aachen University
Turmstraße 46, 52056 Aachen, Germany
Phone: +49 241 80 – 96712
email: marquardt@lpt.rwth–aachen.de

Abstract. A hybrid model of the state of the art domestic hot water storage unit [3], consisting of a stratified storage tank and a countercurrent heat exchanger is presented in this paper, see Figure 1. The fluid in the storage vessel has a certain temperature profile and thus a density gradient which assures the physical principle of stratification. To maintain this stratification, the storage tank is driven with relatively low mass flows and equipped with baffle plates to ensure that the mixing and excitation of agitation–flows in the in– and outflow regions of the tank are minimized. The dynamics of the plant is characterized by discrete–time events due to e.g. tapping or loading events, as well as time–varying spatial temperature profiles which occur in the storage tank and the heat exchanger. Therefore, the derivation of a finite state automaton describing the discrete–time dynamics of the plant is derived. Further, the underlying continuous–time dynamics of the storage tank and heat exchanger is modeled by two interconnected distributed parameter systems, namely a diffusion convection system (DCS) and a transport system with heat exchange. Consequently, the entire plant can be described as a hybrid distributed parameter system [4]. Due to the hyperbolic nature of the DCS, the temporal evolution of steep spatial gradients is subject to numerical investigations, i.e. the performance of various spatial discretization schemes for the convective part of the DCS is observed via numerical simulations. These discretization schemes are applied to the heat exchanger and storage model and numerical simulations are compared with measurement data. It is verified that a high resolution slope limiter scheme with Superbee limiter [2] outperforms an up–/downwind and central difference scheme and proofs to fit the measurement data for tapping and loading very well. Consequently, this model is suitable to study the challenging task of process control design for the stratified storage tank with heat exchanger as an example for a hybrid distributed parameter system [1].

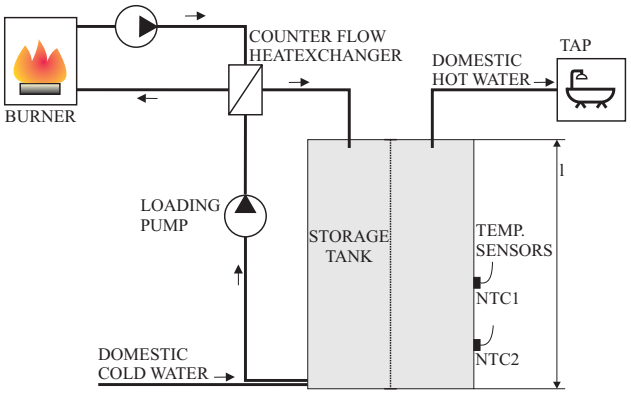

Figure 1: Sketch of the plant.

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[1] Corresponding Author

MODELING OF PIEZOELECTRIC STRUCTURES - A HAMILTONIAN APPROACH

H. Ennsbrunner and K. Schlacher, JKU Linz, Austria

Corresponding Author: H. Ennsbrunner
Institute of Automatic Control and Control Systems Technology
Altenbergerstraße 69, 4040 Linz, Austria
Phone: +43 732 2468 - 9733, Fax: + 43 732 2468 - 9734
email: helmut.ennsbrunner@jku.at

This contribution is dedicated to the geometric description of infinite-dimensional port Hamiltonian systems with in- and output operators and their application to the piezoelectric field equations.
In the first part the used mathematical framework consisting of bundles, jet spaces and related operations is introduced. Thereby the geometric representation of independent and dependent coordinates, but also of partial derivatives of dependent coordinates with respect to independent ones becomes available.
Having this powerful tools at ones disposal, one is able to give a geometric representation of infinite-dimensional port Hamiltonian systems by

$$\begin{aligned} \dot{x} &= (\mathfrak{J} - \mathfrak{R})\left(\delta\left(h_0 \mathrm{dX}\right)\right) + \mathfrak{B}\left(u\right) \\ y &= \mathfrak{B}^*\left(\delta\left(h_0 \mathrm{dX}\right)\right) \ . \end{aligned}$$

The main part of this contribution is dedicated to the detailed specification of all operators $\mathfrak{J}, \mathfrak{R}, \mathfrak{B}, \mathfrak{B}^*, \delta$ as maps between certain vector bundles. This was already done in [Ennsbrunner, K. Schlacher(2005)], but here we assume in addition, that the in- and output operators $\mathfrak{B}, \mathfrak{B}^*$ are certain linear differential operators.
It is shown, that the use of differential operators has major impact on the derivation of the boundary conditions. It turns out that additional boundary ports are introduced by such a configuration.
After these theoretical investigations the piezoelectric field equations are under investigation. This is done by the introduction of a stored energy function e_S

$$\mathrm{d}e_S \wedge \mathrm{dX} = \left(\sigma^{\alpha\beta}\mathrm{d}\varepsilon_{\alpha\beta} - D^{\psi}\mathrm{d}E_{\psi}\right) \wedge \mathrm{dX} \ ,$$

where the stress tensor σ, the strain tensor ε, the electrical field strength E and the electric displacement D is used. Additionally we assume the kinetic energy density e_K to be given by

$$e_K \mathrm{dX} = \frac{1}{2\rho} p_\gamma \delta^{\gamma\eta} p_\eta \mathrm{dX} \ ,$$

whereby the generalized momenta p are introduced. The electrical field strength E is assumed to be the distributed input to the piezoelectric structure. Thus it is only necessary to focus on the mechanical part of the coupled field problem.
It turns out, that certain nonlinear constitutive relations of the form $\sigma^{\alpha\beta}\left(\varepsilon, E\right) = C^{\alpha\beta}\left(\varepsilon\right) - G^{\alpha\beta\psi}E_{\psi}$ allow a port Hamiltonian formulation of the piezoelectric field, as the input acts on the system in a linear fashion.
Finally we obtain from the analysis of the piezoelectric field equations in I-pHd framework a very interesting explanation of the frequently used method of "input shaping" for piezoelectric devices. The existence of a linear differential input operator enables the use of spatial input shapes, such that the input is in the kernel of the domain input operator. Consequently the distributed domain input acts in a similar fashion on the system as a boundary input. This is well known from the modeling and control of piezoelectric beam structures as shown in e.g. [Kugi(2001)].

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FRONT END BENDING CAUSED BY ASYMMETRICAL ROLLING CONDITIONS: AN ANALYTICAL APPROACH

T. Kiefer and A. Kugi, Saarland University, Germany

Corresponding Author: Andreas Kugi,
Chair of System Theory and Automatic Control, Saarland University
P.O. Box 151150, 66041 Saarbrücken, Germany
Phone: +49 (0)681 302-64720, Fax: +49 (0)681 302-64722
email: andreas.kugi@lsr.uni-saarland.de

Front end bending is a phenomenon that occurs in the hot rolling process of heavy plates due to asymmetries in the roll gap like e.g. different circumferential velocities of the work rolls, different friction parameters or a vertical temperature gradient. Due to the form of the bended plate this effect is sometimes also referred to as the ski-effect. The occurrence of this ski-effect has to be avoided because on the one hand the quality of the rolled product is reduced, and on the other hand the ski-ends may even damage the roller table and the measuring equipments near the roll gap. Additionally, ski-ends are known to cause severe problems in the further processing steps, e.g. at the hot straightening machine and in the cooling zone.
In general, the ski-effect can be quantified by the curvature of the outgoing plate ends. The interesting point in the front end bending phenomenon is that the curvature depends not only on the asymmetries themselves but also on the geometry of the roll gap. In particular, it can be shown that for identical asymmetrical rolling conditions the curvature even changes sign when rolling plates of different thicknesses with different thickness reductions. Thereby, the so-called shape factor, i.e. the ratio of the arc length of contact to the medium plate thickness, is usually used to characterize the roll gap geometry. Let us consider the case of a homogeneous plate where the only asymmetry in the roll gap is due to different circumferential velocities of the work rolls. Then, for small shape factors the plate behaves as it would be expected, namely the material tends to bend away from the faster work roll. In contrast to this, for larger shape factors, the curvature changes sign and the plate bends towards the faster work roll, see Fig. 1. Clearly, a mathematical model has to be able to describe all these effects in order to serve as a suitable basis for designing control strategies to avoid front end bending.
Several models for predicting the curvature of the outgoing plate ends can be found in the literature, e.g. based on the slip-line field analysis in [1], on Finite Element (FE) methods in [2] or on the upper bound method in [3], [4]. In general, these models are only of limited use in process control since either the computational costs are too high or the models are not accurate enough to describe the basic phenomena as discussed above. In the present paper, we will present a physically motivated mathematical model also based on the upper bound method for rigid-plastic materials that has proven to be a good compromise between a high degree of accuracy and low computational costs for executing the model in the process control unit.

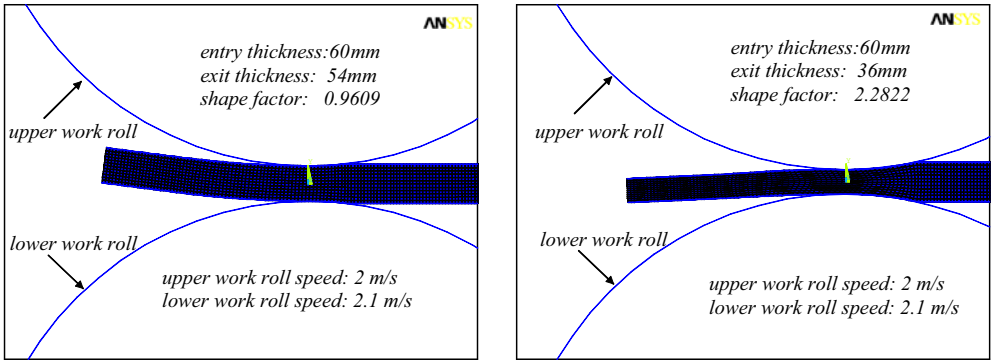

Fig. 1: FE solutions with identical asymmetrical conditions in the roll gap for different shape factors.

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Advanced Mathematical Methods for Simulation Based Research Services

COMPARISON OF PID, IMC AND FUZZY GAIN SCHEDULING CONTROLLERS IN VARYING TIME-DELAY SYSTEMS

L. Eriksson and H. N. Koivo, TKK, Finland

Corresponding Author: L. Eriksson,
Helsinki University of Technology
P.O. Box 5500, FI-02015 TKK, Finland
Phone: + 358 9 451 5231, Fax: + 358 9 451 5208
email: lasse.eriksson@tkk.fi

In the paper a comparison of three different control methods (PID, IMC and fuzzy gain scheduling) is made in varying time-delay systems. The investigated system is modeled as a first order system with a delay. The varying time-delays are either properties of the system or they may be introduced by networks that are used for measuring the system. The paper discusses three delay models: 1) constant delay, 2) random delay, and 3) correlated random delay. Altogether five different controller realizations are compared in this framework. In addition to the controllers, the process and the delay models are implemented in Simulink, and the control performance is evaluated using simulation.

If control is considered, a varying time-delay in the closed-loop is a great challenge. This area has been under extensive research during the last decade because of the interest of using networks in control systems, see [1] - [3]. This study investigates general properties of different control algorithms in varying time-delay systems. Thus two very general varying time-delay models are chosen for the comparison: 1) Gaussian random delay and 2) correlated random delay. Five different control algorithms are chosen for comparison. There are two variations of the PID algorithm and two variations of the IMC controller, and the last controller is a combination of fuzzy gain scheduling and PID controllers.

The simulation results (presented in Fig. 1) suggest that in the Gaussian random delay case the more advanced controllers might not guarantee better performance for the system and the conventional PID or IMC controllers are feasible. But if the delay is somehow correlated, which is often the case in networked control systems, improvements in performance can be achieved with more advanced controllers such as the delay-adaptive IMC controller and the delay-based fuzzy gain scheduling. If the delay variation is insignificant with respect to the process time constant the controllers perform in similar way and the advantage of taking the varying delay into account in the control algorithm diminishes. The more advanced control algorithms require the measuring of the delay, which might sometimes be problematic. Often, the delay can at least be estimated online.

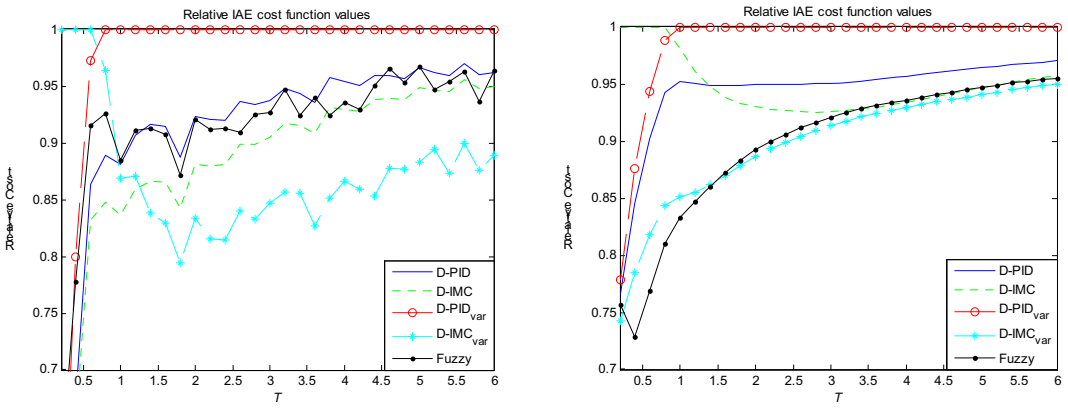

Fig. 1: Relative IAE cost function values for random delay (left) and correlated random delay (right) case.

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SELF-TUNING RECURSIVE MODELLING AND ESTIMATION OF WEATHER MEASUREMENTS

Vesa Hasu, Helsinki University of Technology, Finland
Jani Poutiainen, Finnish Meteorological Institute, Finland
Heikki Koivo, Helsinki University of Technology, Finland

Corresponding Author: V. Hasu,
Control Engineering Laboratory, Helsinki University of Technology.
P.O.Box 5500, 02015 HUT, Finland.
Phone: +358 9 451 5226, Fax: +358 9 451 5208
Email: vesa.hasu@hut.fi

The state of the weather has been, is and will be one of the most popular discussion topics in the history of mankind. In addition to idle conversations, knowing the weather and reacting accordingly can have impact from everyday convenience to enormous economical savings. The recent development of measurement equipment has made possible to measure meteorological phenomena densely in large weather station networks with short measurement interval, thus offering new possibilities in weather analysis and nowcasting. Observations are necessary prerequisites for weather forecast models.

The measurements utilized in this paper are from the Helsinki Testbed -mesoscale measurement network which is led by Finnish Meteorological Institute and Vaisala measurements company. Outcomes from testbeds are more effective observing systems, better use of data in forecasts, improved services, products, and economic/public safety benefits. Testbeds accelerate the translation of research and development findings into better operations, services, and decision-making.

The weather station network has two basic needs for the modelling and estimation. Firstly, the possible noisy measurements can be easily filtered. Such noise can occur due to sensor flaws, a poor installation or weather conditions. Especially weather conditions make the filtering interesting. Distinguishing actual weather phenomena from noise is a difficult task for filtering and estimation. The second need for modelling is the estimation of missing measurements. The absence of measurements can occur *e.g.* due to wireless link mishap, maintenance break or sensor failure. The estimation of missing measurements can be done according to the same measurement history or according to the measurements of the neighbor stations.

Note that the scope of the research is concentrated on the measurements and their quality, not so on the predicting values of meteorological measures for future time steps. Our approach of time series modelling is not accurate at all through the whole nowcasting timeframe of several hours.

The weather measurements are modelled in here as moving average time series model. The model is updated in each iteration by a recursive least squares method (RLS). This model is formatted into state-space representation and used in Kalman-techniques for estimation and prediction purposes. Kalman-techniques are widely covered in the literature.

The Kalman-predictor can compensate the missing measurement values and the Kalman-estimator can smooth out possible excessive noise. The covariance matrices for system and measurement noise required for Kalman filter are estimated recursively. This guarantees the applicability of the model for different measurements in different meteorological conditions, *e.g.* measurements in inland and coastal stations can have very different statistical properties.

The missing measurements can decrease the system performance significantly, if the measurement is missing for a long period and the neighbor stations are far away. A long period with no measurements and the model structure leads to an autoregressive sequence, which is not accurate after a few hours of measurements. Hence additional parallel model structures are applied, in which the missing measurement is removed in RLS model.

CONCURRENT ENGINEERING OF SUBPROCESS MODELS WITH APROS

T. Ollikainen, VTT Technical Research Centre of Finland, Finland; K. Porkholm, Fortum Nuclear Services Ltd, Finland; A. Ahmed, ETCA, Assiut University, Egypt; F.A. Hady, UEEPC, Egypt

Corresponding Author: T. Ollikainen,
VTT Technical Research Centre of Finland
P.O. Box 1000, 02044 VTT, Finland
Phone: +358 20 722 6571, Fax: +358 20 722 7053
Email: toni.ollikainen@vtt.fi

Abstract. Modern simulation software enables fast and accurate modelling of wide entities. The functionalities of process-, automation- and electrical equipments can be all modelled in the same simulation environment. The modelling of different subprocesses can be distributed between different modelling groups including several modellers having expertise on specified parts of the process.

This paper introduces the working method of concurrent engineering used in the modelling of large scale industrial processes with APROS (Advanced PRocess Simulator) software. It has been widely used for process and automation design, safety analysis, operator training and I&C system testing. The modelling is done through a graphical user interface by specifying the process, automation and electrical diagrams and introducing the required parameters to the included process, automation and electrical component models. The modelling work is straightforward based on the initial data of the simulating process. A skilled modeller can develop an accurate simulation model for a power plant in a couple of months. The time used for the development of a simulation model is often critical. This working time and the delivery time can be decreased by dividing the simulation work between several modelling groups and modellers. The concurrent engineering method makes the development of the simulation model more effective due to the fact that the modellers really can concentrate on the expertise they have on specific subprocesses. The concurrent engineering sets new requirements for the management of the simulation project. The utilization of the method can reduce remarkable the model development time, which enables to take into use the simulation considerably earlier in the project. Strict version control has to be employed in modelling project involving extensive processes. All changes introduced to the models have to be documented in detail. Efficient simulation platforms and version control tools or methods are required.

An example of the described method in practise and the experiences of the modelling project are illustrated in the paper. The case presented in the paper shows the benefits of the presented method. In the case a basic simulation model of the second unit of New Assiut Thermal Power Plant (2×325 MW was built, in February 2005 at the site of ETCA in Assiut, Egypt. The plant is a conventional oil-fuelled power plant that has a steam turbine producing a power of 325 MW. The simulation model was designed especially for the training purposes of the drum-boiler dynamics and process air-fuel ratio changes as well as the functionality of the control system. All the necessary level controllers were included in the basic model. The modelling work was accomplished with presented method by two separate teams within one week.

One of the experiences gained by the operating engineers of the plant is to use APROS software to adjust the air/fuel ratio such that the emissions from the stack outlet point remains within the levels safe to the environment, which constitutes one of the challenges facing such thermal power plants.

SYSTEM DYNAMICS – A TOOL FOR DESIGNING AND ANALYSING COMPLEX PROCESSES

J.-P. Ylén and V. Hölttä

Corresponding Author: J.-P. Ylén
VTT Technical Research Centre of Finland
P.O.Box 1301, FI-02044, VTT, Finland
Phone: +358 40 507 7474, Fax: +358 20 722 7053
email: peter.ylen@vtt.fi

In recent times there has been a lot of interest on system dynamics modelling, a concept first introduced by MIT professor J. W. Forrester in the 1950s. The increase of computing power and advance of computers has enabled the analysis and simulation of many large scale systems. There are several commercial tools with easy-to-use graphical user interfaces available in the field of system dynamics. These commercial tools are briefly discussed in this paper. In addition to describing the tools, this paper gives a short introduction to system dynamics models and their capabilities with simple examples.

In effect, system dynamics is merely the art of applying dynamic models to practical systems, e.g., decision making and production processes. Systems described by system dynamics models are typically large, complex, nonlinear sets of differential equations. Theoretical system analysis usually fails in these cases, mainly because linear approximations cannot be used. Top-line structural analysis can be performed (such as analysis of dominating positive and negative feedback loops and their interactions) but theoretical analysis is beyond the grasp of the modeller.

The structure of the system dynamics model is a loop diagram, which consists of simple positive and negative feedback loops. A typical positive feedback loop is a population growth: larger population generates more births, which results even larger population and even more births, etc. This is shown in a simple loop diagram in Fig. 1

It is just as easy to find a simple negative feedback loop limiting the population explosion. Let us consider that there is limited amount of food available. The carrying capacity of that area limits the population growth. Large population consumes a lot of food leaving less food per capita, this causes starvation, deceases and death, which makes the population smaller and then there is again more food per capita, etc. (See Fig. 2.)

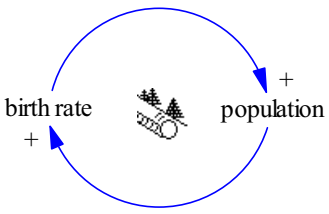

Fig. 1. A simple positive feedback loop

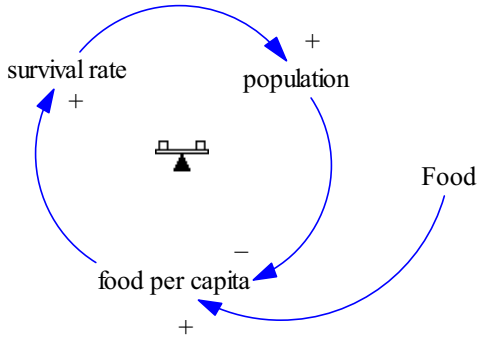

Fig. 2. A simple negative feedback loop.

The system dynamic models can be simulated with any simulation tool, but there are a couple of software tools specifically designed for system dynamic applications. They have a library of typical models, a number of analysis tools, such as, dominant loop analysis and sensitivity analysis and the results are presented in an easily digestible format. Currently, there are three major tools at the market: Vensim, Powersim and ithink.

There is active research going on and the number of industrial applications is increasing rapidly. The commercial tools are improving and different analysis and design tools within these commercial products are developing significantly. As a result the amount of tedious hand work needed for system dynamics modelling is reducing rapidly and the modelling process is becoming faster and faster.

SOLVING MATRIX EQUATIONS IN LARGE-SCALE DYNAMIC SIMULATION OF FLOW NETWORKS

A. Villberg and T. Karhela, Technical Research Centre of Finland, Finland

Corresponding Author: A. Villberg
Technical Research Centre of Finland
Technical Research Centre of Finland, P.O.Box, 1301, FIN-02044 VTT
Phone: +358407036459, Fax +358406822274
email: antti.villberg@vtt.fi

Dynamic simulation of large-scale flow networks involves computing an approximation for the solution of the corresponding equation of motion. The problem can be reduced to a linear equation system solution using discretisation and linearization of the resulting equations. This paper studies the solution methods for the resulting matrix equation $Ax = b$. Matrix A is generated according to the companion model approach suggested by Juslin [1].

The flow network is divided into nodes and branches. In the example hydraulic circuits a staggered grid discretisation approach is used in which pressures are calculated in nodes and mass flows in branches. Typically a node variable depends on a small number of other node variables and thus the produced matrices are sparse and can be easily solved with a direct factorisation method. More complex processes, which utilise for example major cycles introduce more complex interdependencies, which make direct solution of the equations less feasible.

A performance analysis of a direct factorisation method and an iterative method is presented. The factorisation method has been successfully used in simulation of power networks and industrial processes. This study compares the characteristic behavior of the methods with different modelling scenarios and searches for modelling cases, where an iterative solution method performs equally or superior to the direct solution.

The simulation algorithm used with the companion model approach uses iteration of the matrix solution on two levels. For each time step the matrix solution is iterated because the used approximation of the equation of motion is nonlinear. Importantly the solution vector converges to a solution for the current simulation time. The second level of iteration is over time, with initial solution from last time step already near the solution. In the iterations the matrix structure does not change, but the elements will. The implications of the iteration scheme for different matrix solution methods are studied.

The sparsity of the matrices in consideration has a central role in determining the performance of the solution methods. For the direct factorisation method the sparsity of the factorised matrix is critical as the method is fast only on sparse factorisations. The performance of a reordering procedure in optimisation of the factorisation order is analysed. When the factorised matrices become denser an iterative solver becomes more attractive. This study looks into situations, where the reordering scheme is unable to prevent large scale fill-up of the factorised matrix.

For the iterative solution convergence time is a central question and the effects of input model structure and preconditioning are studied. Preconditioning plays a major role in the performance of iterative matrix solution methods, but the scope of this study does not include significant analysis of effective preconditioners.

There are different ways in which a process model can grow in size. The performance of the matrix solution methods with respect to input size is analysed with different types of sources for input data.

For general comparison a set of common scalable sparse matrix structures are used as well as matrices arising from instances of real companion model simulation with different parameterisation.

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Efficient Operation of Sequential Batch Reactors for Wastewater Treatment

EXPERIMENTS FOR MODELLING THE BIODEGRADATION OF WASTEWATER IN SEQUENCING BATCH REACTORS

G. Buitrón[1], R. Canziani[2], M. Torrijos[3], S. Gutiérrez[4], I. Moreno-Andrade[1], D. Mazouni[3], N. Fiocchi[2] E. Ficara[2], G. Moreno[1], A. Benitez[4], J. Pérez[1], A. Ferrari[4]

Corresponding Autor: G. Buitrón
[1] Universidad Nacional Autónoma de México (UNAM), Instituto de Ingeniería, Circuito Interior, Ciudad Universitaria, 04510 Mexico D.F., Mexico. Email: gbm@pumas.ii.unam.mx
[2]Politecnico di Milano (POLIMI), Department of Hydraulics Environmental Infrastructure and Survey Engineering- Environmental Section, Piazza Leonardo da Vinci 32, I-20133 Milano, Italy. Email: roberto.canziani@polimi.it
[3]Institut National de la Recherche Agronomique (INRA), Laboratoire de Biotechnologie de l'Environnement, 2, Avenue des Etangs, 11100 Narbonne, France. Email: torrijos@inra.ensam.fr
[4]Universidad de la República Oriental del Uruguay (UU), Instituto de Ingeniería Eléctrica - Facultad de Ingeniería, Julio Herrera y Reissig 565, 11200 Montevideo, Uruguay. Email: Soledadg@fing.edu.uy

Abstract
The aerobic treatment of wastewaters by activated sludge is a common process, but the characteristics of many industrial discharges often cause operational problems in continuous flow systems. Therefore, the discontinuous processes, as sequencing batch reactors (SBRs), were considered in this project because, in terms of investment and operation costs, process stability, and operation reliability, they are better than the conventional continuous activated sludge process. The benefits of the SBRs have been shown for nutrient removal, the control of filamentous bacteria and the removal of specific organic compounds present in industrial wastewaters.

The objective of the EOLI project is to design a low-cost, modular and reliable monitoring and control system for wastewater treatment process dedicated to the treatment of wastewater from urban settlements, especially from those urbanized areas where industries contribute heavily to water pollution. In this project three cases of wastewaters were considered: a municipal wastewater, the effluent of a dairy industry, both polluted with organic carbon and nitrogen, and a wastewater typical of a chemical industry, containing toxic or recalcitrant compounds. For this case, a synthetic wastewater contaminated with a 4-chlorophenol was used.

In the study, laboratory and field-scale pilot reactors were used. At the start of the project, process experiments were performed to provide experimental data for parameter identification of the dynamical models of the SBRs. An experimental protocol was defined in order to optimize the information content of the data for parameter identification while accounting for the different process constraints. Then, the experiments were carried out to test the different outcomes of the project (hardware sensors, software sensors, control laws, FDI, supervision system). SBRs were instrumented with sensors to measure O_2, NH_3, T, pH, OUR, and other off line measurements (e.g.: NO_2^- and NO_3^-, COD, phenol concentration, microbiological counts and activities) in order to study more accurately the behaviour of the biomasses. However, the general idea is to design a system with the minimal number of sensors.

A set of data was obtained in order to calibrate and validate a model for SBR systems fed with crude and pre-treated municipal and dairy wastewater in anoxic and aerobic phases. Results showed that experiments were coherent with the mechanistic knowledge of the basic biological processes taking place in the SBR. Data concerning the sludge settling will be used to develop a supervision algorithm to monitor the settling phase and to avoid a bad settleability in the SBR. Basic information on the biological behavior can be obtained from on-line signals (DO, pH and ORP), although they are more qualitative then quantitative. The need for on-line systems allowing plant operators to have early-warning information on the quality of the influent to be treated, allowing for effective plant operation, would greatly improve process efficiency.

The biodegradation of a toxic wastewater containing 4CP as model of an inhibitory compound was obtained. A good performance of the reactor operated with the optimal control strategy was obtained since the degradation of the 4CP was efficiently completed (99%, as chemical oxygen demand, and 100% as 4CP). The optimal strategy was also able to manage increments of toxicant concentrations in the influent up to 613 mg 4CP/L. There was not a significant influence on the performance when the air inflow rate was varied ±50% with respect to the standard condition.

Dynamical modelling, identification and software sensors for SBRs

H. Fibrianto*, D. Mazouni+, M. Ignatova**, M. Herveau+,
J. Harmand+ and D. Dochain*

* : CESAME, Université Catholique de Louvain
4-6 av. Georges Lemaître, B-1348 Louvain-la-Neuve, Belgium
+ : LBE-INRA, avenue des étangs, F-11100 Narbonne, France
** : ICSR, BAS, P.O.Box 79, 1113 Sofia Bulgaria

Abstract

Within the EOLI project, two different types of models have been proposed to represent the dynamics of two different types of processes. These models have been calibrated and validated on experimental data obtained from the different experimental processes. The first model, referred as EM1, corresponds to the process run in Mexico. The second model represent the dynamics of the processes run at POLIMI, at the LBE and at the UU. Due to slight differences between the process dynamics, two submodels have been identified, i.e. EM2a for the POLIMI process, and EM2b for the LBE process. The models as they are presented here are indeed the result of an iterative process between model building and process experiments. If the main frame of the models have been built in the initial step on the basis of the partners' experience and of the available scientific literature of the subject, several modifications have been included at the light of the physical/(bio)chemical evidences provided by the experiments. This has resulted in the design of extra experiments in order to validate the new modelling assumptions.

In this paper, we concentrate on models EM1 and EM2b, which are considered in the second part of the paper for the design of software sensors. In the paper only the reaction schemes, the mass balance equations (with the kinetic expresssions), the basic identification procedure and the parameter values are provided. Details about the identification procedures for the different models can be found in the related more detailed project reports. The identified models have been used for several purposes in the project : software sensor design, FDI, and control design. In the present manuscript, we concentrate the software sensor design results. As for any biotechnological processes, the on-line monitoring and control of the SBR's is facing two major difficulties : the lack of measuring devices that can provide the values of all the key process components on-line, and the lack of confidence in the dynamical models of the processes (even with our quite careful identification procedure). This motivates to design software sensors that are capable of providing reliable software measurement (estimates) of the key components in spite of the model uncertainty that is typically mainly concentrated in the process kinetics.

Development of hardware sensors for the on-line monitoring of SBR used for the treatment of industrial wastewaters

Roberto Canziani, Elena Ficara, Nicola Fiocchi, *Politecnico di Milano, Italy*
Paolo Ratini, Massimiliano Pirani, Simone Mariani, *SPES, Italy*
Meriem Bekri, André Pauss, Thierry Ribeiro, Olivier Schoefs, *Université de Technologie de Compiègne, France*
Jean-Claude Bouvier, Jérôme Harmand, Djalel Mazouni, *LBE- INRA, Narbonne, France*

The main challenge in the management of a sequencing batch reactor, for the biological treatment of urban and industrial wastewaters, is to ensure a stable treatment efficiency under highly variable influent quality and quantity. To cope with this challenge, on-line instrumentation is fundamental, since it allows to characterize both influent variability and process efficiency. The more the on-line data are closely correlated with influent quality and SBRs treatment capacity, the more straightforward is to implement control strategies based on these data.

Set-point titration

Set point titration allows the assessment of two kind of information of great interest in the monitoring of SBRs:

- treatability of the influent, in terms of sewage toxicity to the biomass and pollution load;
- the biomass treatment capacity, in terms of process rate.

The following procedures, or modes, have been developed and experimented:
1) detection of influent acute toxicity to nitrifying biomass; 2) estimation of the influent nitrifiable nitrogen content; 3) measurement of the nitrification capacity of the SBR, assessed in terms of maximum rates of oxidation of ammonium to nitrite and of nitrite to nitrate, allowing to predict nitrite build up; 4) monitoring of ammonium oxidation process during the aerobic react phase of the SBR reactor; 5) estimation of nitrate concentration.
Measuring procedures and results will be presented, as they have been implemented by an at-line automated titrator (TITAAN, TITrimetric Automated ANalyser) at two pilot-scale SBRs.

UV-Spectrometry

The UV spectra is linked to the absorbance of non-binding electrons in molecules, and to the diffusion of light by suspended solids and colloid in the liquid solution. The absorbance is proportional to compound concentrations, but the UV spectrum shapes are quite wide, and their specificities are often low due to the number of close absorbance rays.
Therefore, UV spectra are often used as it to handle the qualitative evolution of an effluent, with a special focus to one or more specific wavelengths. Spectra are understood as fingerprints of specific wastewaters, whose variations by time are essentially considered It is however possible to be ahead of the qualitative aspects using decomposition techniques.
Two decomposition techniques were tested, a PLS regression and those used by the UV-Pro software (Secomam company). High correlation coefficients (>0.95) were obtained for nitrate, nitrite and organic substances, comparing experimental and estimated values for 28 tests. After this calibration, validation was successfully performed on the pilot scale SBR in Narbonne. An on-line spectrophotometer sensor was developped and implemented on the pilot scale.

Conclusions

Set-point titration can be applied to SBR for nitrification and denitrification monitoring without classical analytical determination
SBR processes can be monitored with UV spectrometry, as continuous processes, after calibration and validation steps

OPTIMAL CONTROL OF BIOLOGICAL SBRS FOR THE TREATMENT OF DAIRY AND TOXIC WASTEWATERS

M. J. Betancur[2], D. Mazouni[1], J. Harmand[1] and J. A. Moreno[2]

[1]Laboratoire de Biotechnologie de l'Environnement, Institut National de la Recherche Agronomique,
Avenue des étangs, 11100 Narbonne, France.
harmand@ensam.inra.fr, fax: (+33) 468.425.160,tel: (+33) 468.425.159

[2]Institute of Engineering, National University of Mexico, Ciudad Universitaria, Mexico DF, Mexico.

ABSTRACT

The objectives of the control module which was developed within the EOLI integrated system were twofold. First, develop an algorithm for the optimal control of the SBR in the presence of an inhibiting reaction scheme and second, develop a time optimal control strategy for the control of aerobic SBRs with carbon and nitrogen removal capacities.

These model-based control laws are directly derived from the models proposed in (Mazouni et al, 2005). They also take into account the information about for direct measurement (via hardware sensors) presented in (Pauss et al, 2005) and, about the indirect measurement (via software sensors) proposed in (Fibrianto et al, 2006). Because of the type of operation (which is a batch), optimal control is the core of the control design in order to optimise: i) the feeding strategy by distributing the feed with time in order to avoid accumulation of toxics and/or inhibitory substances in the cases of toxic effluents and ii) the aerobic and anoxic phase time durations in order to minimise the total reaction time in the case of carbon and nitrogen removal.

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DETECTION OF ABNORMAL CONDITIONS OF AN AEROBIC SBR PROCESS USING FEATURE EXTRACTION

D. Wimberger and C. Verde Rodarte, IINGEN, UNAM, México

Corresponding Author: D. Wimberger
Instituto de Ingeniería, Universidad Nacional Autonoma de México
Edificio 12, Circuito Exterior, Coyoacán 04510 México DF
Phone: +52-(55)-56233683, Fax: +52-(55)-56233681
email: dwimbergerm@iingen.unam.mx

Sequencing Batch Reactors (SBR) for waste water treatment (WWT) based on the fill-and-draw principle [1] are commonly employed to deal with variations in flow and composition of residual waters. For autonomous operation, these batch processes require a control system that maintains the operation even under presence of faults. To achieve this goal, the process has to be permanently monitored to detect the presence of faults, diagnose their type and size [3] and take corresponding actions. This is an especially critical feature in the case of the presented study about an aerobic SBR activated sludge waste water treatment (WWT) process treating water contaminated with organic toxic compounds.

The main requirement of data based PFD is that data is available and accompanied by diagnostic information. While in many cases historical data from operations is the main source, it is also possible to generate data and diagnostic information using an uncertain mathematical model. Given the absence of sufficient historical data, a process model is introduced and transformed so that a continuous online estimate of the respiration rate during the SBR reaction phase with feeding can be obtained. This process signal has been widely recognized as an indicator for biological activity and employed for monitoring and control purposes [4].

The usefulness of the signal for the detection and classification of a set of defined abnormal conditions (eg. process faults) is verified through sensibility analysis [2]. Results from this analysis not only show the effects of parameter deviations, but also indicate the features that should be extracted from the respiration signal for a successful classification. Consequently a feature extraction and classification procedure is proposed, that is designed to diagnose the formerly defined process faults. In spite of significant uncertainties the methodology is proven to be quite successful, given that the percentage of correct detection and diagnosis is above 95% in almost all cases. This indicates that the machine learned classification models can be used online for the detection and diagnosis of certain process faults, which cannot be detected by a straightforward application of well studied quantitative PFD approaches.

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DEVELOPMENT OF AN INTEGRATED SYSTEM FOR THE OPTIMISATION OF SBR'S

P. Ratini, M. Pirani, S. Mariani, A. Quintabà, L. Luccarini, D. Mazouni, N. Fiocchi and J. Harmand

Abstract

The EOLI project aimed at developing an integrated system for the on-line optimization of biological SBR processes treating urban and industrial (including toxic) wastewaters. As a demonstration example, in a first part, this paper presents the advanced framework of the supervision system which has been developed to manage the reaction phase of an aerobic SBR treating dairy wastewaters. In a second part, both hardware and software capabilities of the EOLI integrated systems are presented.

The EOLI Decision Support System (DSS) is completely modular. A number of different modules have been developed with respect to the actual available instrumentation. To summarize, three supervision levels distinct modules have been proposed :

- An industrial DSS including the signal processing modules when a low instrumentation is available : this system is suitable when only DO/Redox potential and/or pH measurements are installed on the system. This module is presented elsewhere.
- A DSS able to deal with qualitative and quantitative information delivered by advanced instrumentation including Titrimetric sensors such as MARTINA, Biosensors such as TITAAN or UV sensors.
- A specific DSS devoted to the management of the sludge settling capabilities.

Taking into account the information provided by the TITAAN and/or by the UV sensor that have been developed within the framework of EOLI, the basic idea of the actual supervision system is to perform on-line a mass balance on the carbon and on the nitrogen. In other words, the idea is to verify if the actual oxygen consumption fits the theoretical oxygen needs with respect to the available knowledge about the yields of the different involved bioreactions. The balance which is realized is based on the following calculations.

Within the project, there are several wastewater treatment plants that are being fitted with the EOLI system, adapted to their individual needs. These are the project's integrated systems. Integration means the setting up and basic testing of the EOLI modules on a SBR plant site, within the framework - the middleware - that allows them to communicate with each other and with the SBR process itself. The integration activity involves two real physical plants with the aim at validating the reliability and customisability of the system: the pilot scale plant at ENEA (Italy), and the pilot- scale plant at INRA (France). These plants have very different characteristics, and thus it is an effective test for the EOLI approach to be able to integrate them all within the same framework.

The whole integrated system produced at the end of the project is characterised by the high level of modularity pursued for the integration that makes it possible to configure, to enroll, to enable or to disable all the possibly numerous components. Therefore the system can be applied at plant of different size, under different sensors network configurations. The experience from the installation, running and maintenance at two different pilot plants, the ENEA and the INRA ones, confirm this result. The full customisability, that was a key requirement for the development of the system, is a consequence of this high and reliable modularity.

In order to test and to demonstrate the potentialities and capability of the EOLI system as far as the data management and integration, other three plants located out of Europe, the IbTech full scale plant in Mexico and the two lab plants at University of Uruguay have been logged to the EOLI remote server.
These plants have to be considered as examples of architectures compliant with the EOLI software supervision system, equipped with monitoring and control systems built up with off the shelf solution. This enforces the policy for exploitation and dissemination of the results of the EOLI project: the software main frame and the whole monitoring and control systems developed provide general features and capabilities that are customisable to many other types of EOLI compliant installations.

The EOLI project is based on the idea that each remote WWTP is connected to a Remote Server Machine – located at a remote control centre - in order to upload measured data and alarms and download control actions. This Remote Server is essentially a supervisor system which implements a distributed control architecture. It has been chosen to use Internet as the main connection infrastructure between the Remote Server and each plant; this is because of the flexible, inexpensive and widespread nature of this medium.
The core, both at the remote control centre and at the local plant, is a relational database and it is used to store all the data gathered (measurements), generated (commands), transferred and managed by the EOLI system.
The EOLI software architecture is based on the client/server technology in which different modules implemented for different purposes, can share the same resources using a relational database management system (DBMS) that is introduced to replace the limitations of the file sharing architecture: the client/server technology is a versatile, message-based and modular infrastructure that is intended to improve usability, flexibility, interoperability and scalability.

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Object Oriented Modelling in Mechatronics

OBJECT-ORIENTED MODELLING OF TWO-PHASE FLUID FLOWS BY THE FINITE VOLUME METHOD

F. Casella, Politecnico di Milano, Italy

Corresponding Author: F. Casella
Dipartimento di Elettronica e Informazione
Politecnico di Milano
Piazza Leonardo da Vinci 32, 20133 Milano, Italy
Phone: + 39 02 2399 3465, Fax: + 39 02 2399 3412
email: francesco.casella@polimi.it

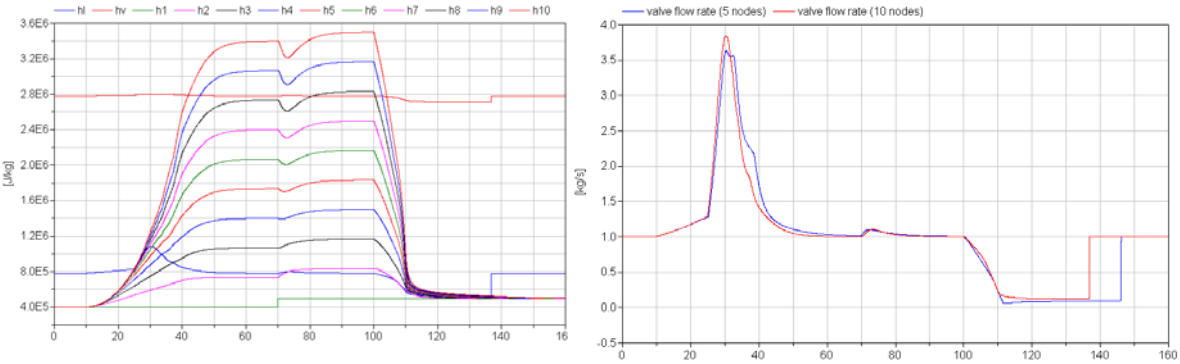
Dynamic modelling and simulation of thermo-hydraulic systems can play an essential role in the design of control systems for energy conversion plants. Object-oriented modelling techniques, in particular the Modelica language [1], are increasingly being used in this field, thanks to their flexibility and ease of use.

Two-phase fluid flows are often encountered in energy system. Their simulation in the context of control system analysis and design requires an appropriate degree of complexity, so that lightweight models are obtained, giving a fairly good representation of control-relevant dynamics.

Most existing general-purpose Modelica libraries dealing with thermo-hydraulic dynamics (e.g. ThermoFluid [2]) include fairly accurate finite-volume 1-dimensional models of fluid flows in pipes, which are however based on the hypothesis that the fluid properties do not change too drastically across each of the finite volumes. This hypothesis does not hold when two-phase conditions are established, as it happens, e.g., in evaporators; strong discontinuities arise in volumes containing a phase change boundary. As a consequence, unwanted numerical artefacts are generated whenever a two-phase boundary crosses one of the finite volume boundaries.

This paper present a mathematical model, based on the finite volume method, which completely avoids those artefacts, thus allowing to use a limited number of nodes in evaporator models, to meet the needs of control-oriented simulation. The resulting model equations are continuously differentiable even when the two-phase boundaries cross the discretization nodes, avoiding numerical artefacts, and allowing numerical integration by high-order and/or multi-step methods. The model has been included in the Modelica library ThermoPower [3].

The simulation of a simple test case, resembling a once-through boiler, demonstrates the potential of the model. The two figures show the transients of specific enthalpy and outlet flow rate corresponding to an increase of heat flux, followed by a step increase of the inlet enthalpy, followed by a reduction of the heat flux.



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MODELLING AND SIMULATION OF MOTORCYCLE DYNAMICS FOR ACTIVE CONTROL SYSTEM PROTOTYPING

G. Ferretti, S.M. Savaresi, F. Schiavo and M. Tanelli, Politecnico di Milano, Italy

Corresponding Author: G. Ferretti
Politecnico di Milano
Piazza L. Da Vinci 32, 20133 Milan, Italy
Phone: +39 02 2399-3682, Fax: +39 02 2399-3412
email: ferretti@elet.polimi.it

This paper presents a simulation model for the dynamic behavior of a motorcycle developed in Modelica, within the Dymola environment. Dymola, based on the acausal object-oriented language Modelica, is a state-of-the-art simulation tool, allowing a fully modular approach to physical system modelling and featuring advanced symbolic manipulation techniques and numerical solvers for non-linear Differential-Algebraic Equations (DAE) systems.
The motorcycle model is tailored to be employed for test and validation of active control systems for motorcycle dynamics. To design a control oriented simulator for two-wheeled vehicles is a very challenging task, as a complete analytical model is not directly available due to its complexity and its high sensitivity to parameters' variations. Accordingly, a reliable model should be based on multibody modeling tools endowed with automated symbolic manipulation capabilities.
The core of an effective motorcycle simulator, though, lies in tire modeling and in managing the interaction between tires and road, which has a major impact on both ride and handling properties of motorcycles. In fact, the tire allows contact between the rigid part of the wheel – the hub – and the road surface to take place on all surfaces and in every road condition. Moreover, the tire is the means for ensuring adherence to the road and it is responsible for transferring to the ground the vertical load, which is decomposed – in the contact plane – into longitudinal (*i.e.,* traction and braking) and lateral friction forces, which guarantee steerability.
As far as control systems design is concerned, dealing with motorcycle dynamics is far more subtle than it is for 4-wheeled vehicles. In fact, it is well known that most active control systems for cars are commonly developed based on simplified dynamical models (e.g. the quarter car model for braking control systems or the bicycle model for active suspensions control), while complete vehicle models are employed mostly for testing and validation phases. Such design procedure, unfortunately, seems not to fit when moving to 2-wheeled vehicles: the presence of a single axle does not allow to resort to simplified models, and the tire-road interactions effects can never be disregarded, not even during a first analysis phase. In fact, one has to handle strong dynamic coupling between the rigid bodies (front and rear frames, front and rear wheels) and the elastic joints (fork and front and rear suspensions), which make it difficult to devise appropriate reduced model for control purposes. The effort of analyzing well-defined driving conditions on a complete dynamic simulation model seems to be the key for a comprehensive control design for motorcycles. Such approach is well confirmed in the available literature.
But maybe the main crucial difference between cars and motorcycle dynamics is due to the driver impact: while in a 4-wheeled vehicle the effects of the driver on the system dynamics can be simply regarded as a measurable disturbance (*i.e.*, the steering angle), in a motorcycle the driver behavior, in terms of its current position and mass distribution during the ride, is a key (yet not measurable) variable for defining the vehicle istantaneous center of gravity. Our model, up to now, treats the driver as an additional mass rigidly connected to the vehicle center of gravity, but we are working to insert the driver lean angle as an additional degree of freedom in the motorcycle model, in order to fully capture the real driving behavior and its effects on the overall vehicle dynamics.

Object Oriented Modelling and Simulation of Parabolic Trough Collectors with MODELICA

L.J. Yebra (C.I.E.M.A.T., Spain), M. Berenguel (U. of Almería, Spain),
E. Zarza (C.I.E.M.A.T., Spain) and S. Dormido (U.N.E.D., Spain)

Corresponding Author: Luis J. Yebra
C.I.E.M.A.T.
Ctra. de Senés s/n. Tabernas. E04200 Almería. Spain.
Phone: +34 950 387923 Fax: +34 950 365015
E-mail:luis.yebra@psa.es

Abstract

This paper presents the actual status of the research performed within the framework of modelling and simulation of Parabolic Trough Collectors (PTC) in the scope of Solar Power Plants. The work is mainly oriented to the development of dynamic models of solar energy plants to be used in the design of automatic control systems aimed at optimizing global performance.

The system used as test-bed plant is the DISS facility, a row arrangement formed by eleven PTCs of 500 m total length, working as a 1 MW_t solar power plant belonging to CIEMAT (Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas - *Research Centre for Energy, Environment and Technology*). A joint project is being carried out in order to develop models and control systems to automatically control these kind of plants.

The final objective of the model is to predict the transient behavior of the thermodynamic variables associated to the thermo-hydraulic output power of the DISS plant (temperature, pressure, specific enthalpy, etc.), when the external disturbances (concentrated solar radiation, ambient temperature, wind speed and direction, etc.) and controllable inputs change.

Due to the fact that the main phenomena are related to thermofluids, the Modelica language has been used to develop these models including the ThermoFluid library ([3],[1]), as base library over which create our final component models. The authors believe that this library is an important reference in the framework of object oriented modelling of thermofluid systems with Modelica.

The work analyzes the main components of the water-steam thermohydraulic circuit and explains the modelling assumptions, trying to justify each one. Each assumption is oriented to get, by means of the symbolic manipulations that Dymola tool performs, a not high index DAE system for the complete model in which the number of nonlinear algebraic loops is minimized. For this purpose, all the components are classified, following the modelling methodology derived from the Finite Volume Method (FVM) [2], in Control Volumes (CV in ThermoFluid nomenclature) and Flow Models (FM in ThermoFluid nomenclature). In some cases information about the future control system architecture to be implemented is introduced in the modelling phase. An example of components that are modelled using this type of information are the pump and injectors in the subcooled circuit, in which a cascade control plus feedforward [4] will help avoid the multivariate nonlinear dependence of the constitutive equations and let consider them like quasi ideal flow rate generators.

Due to the existence of components whose internal implementation varies in function of modelling hypotheses, the polymorphism and the Modelica language constructs *replaceable/redeclare* has been specially used in some of them, for example in the PTCs.

Finally, simulation results are presented with boundary conditions (controlled variables and disturbances) from actual experiments performed in the DISS plant. Comparisons of up to date calibrated model simulations versus plant measurements are presented and commented.

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MODELLING, SIMULATION AND CONTROL OF SPACECRAFT WITH FLEXIBLE APPENDAGES

F. Schiavo and M. Lovera, Politecnico di Milano, Italy

Corresponding Author: Marco Lovera,
Dipartimento di Elettronica e Informazione, Politecnico di Milano
32, Piazza Leonardo da Vinci, 20133 Milano, Italy
Phone: +39 02 2399-3592, Fax: + 39 02 2399-3412
email: lovera@elet.polimi.it

The attitude and orbit control subsystems (AOCS) play a fundamental role in the operation of modern spacecraft. In recent years, the increasing level of performance expected from satellite platform is resulting in an increasing need for efficient design tools in every domain involved in spacecraft design, and particularly in the area of control oriented modelling and simulation. In particular, as the specifications in terms of bandwidth for attitude control systems become more and more stringent, the classical design assumption of a rigid body spacecraft becomes less and less acceptable and the designer is faced with the difficult task of dealing with structural dynamics of the satellite in the development of the attitude and orbit control laws (see, e.g., [1] and the references therein). While there is now a wide body of literature on the design of control laws for flexible space structures, there seems to be significant room for improvement on the modelling and simulation side, as, to our best knowledge, there a is a lack of dedicated modelling and simulation tools which can deal in an efficient way with such issues.
The development of a spacecraft simulation library based on the use of the Modelica language was started a few years ago (see [2]). The library has already been applied in the investigation of the control problems associated with the use of control moment gyros as primary actuators for attitude control (see [5]). While the library was initially developed as a stand-alone effort, it is now being modified in order to make it compatible with the Modelica Multibody Library (see [4]) and exploit, in the object-oriented modelling spirit, the already available modelling tools for the mechanical part of the system. Among other things, this new approach makes it possible to apply some recent developments in the modelling of flexible bodies in a multibody framework (see [6]) to arrive at a complete object-oriented model of a spacecraft with flexible appendages.
As was previously mentioned, flexible dynamics give rise to significant issues for control design problems. In particular, the first application of the derived models for flexible spacecraft has been the closed loop simulation of a flexible satellite equipped with magnetic torquers as primary attitude control actuators, in order to verify the performance level which can be achieved by means of simple PD-like control algorithms originally developed under the rigid body assumption (see [3]).

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AUTOMATING THE SELECTION OF NUMERICAL SOLVERS

Peter Bunus
Department of Computer and Information Science,
Linköping University,
SE 581-83, Linköping, Sweden
email: petbu@ida.liu.se

Problem solving in science and engineering often requires numerical solution of large systems of equations. It is a common practice today to use off-the-shelf software for solving numerical problems. This trend is supported by the availability of large general purpose mathematical subroutine libraries such as NAG library, LAPACK, Harwell Subroutine Library, PORT Subroutine Library or the Collected Algorithms published by the journal *ACM Transactions On Mathematical Software* and the *Numerical Recipes* published by Cambridge University Press, just to name a few of them.

Selecting the right numerical solver or the most appropriate numerical package for a particular simulation problem it is increasingly difficult for users without an extensive mathematical background and deeper knowledge in numerical analysis. The use of readily available numerical routines poses several difficulties to a normal user:

- Although standard numerical codes usually offer very high quality if used alone, the integrated use together with other software components seldom leads to optimal solutions. Many numerical packages are nested within each other. Hence, the user of an engineering modeling environment has to fiddle with numerical details he/she is neither interested in nor seldom an expert.
- In order to ensure robustness, the tuning parameters of the individual numerical solvers must be made available to the user. This often leads to a clumsy and hardly intuitive user interface thus seriously interfering with the application problem the user is really interested. The available documentation for mathematical software tends to overwhelm users with a multitude of choices and does not provide much guidance in how to make those choices.
- The efficiency of numerical simulation is strongly influenced by a correct choice of the numerical method. This choice can be only made by a knowledgeable user and selecting a well suited mathematical package require a deep understanding of the problem that need to be solve and a familiarity with the available mathematical packages.

In order to overcome some of the above mentioned problemsns, it is a common practice today to use modeling and simulation environments that help engineers to create models through a graphical user interface or by writing custom modeling source code using a high level mathematical modeling language. However, this approach, adopted by simulation environments such as MATLAB/Simulink, gPROMS or Dymola offers a high flexibility at the model input level it is not flexible enough at the simulation level. The user is required to specify in advance the choice of a numerical solver that should be used in combination with a certain simulation model. In some cases, this means that the users need to have advanced numerical analysis knowledge as well a good insight into the structural and behavioral properties of the model to be simulated.

Developing an efficient back-end for simulation environments that accommodates various existing numerical packages (often written in various languages) is a challenging and error prone task. This paper introduces, ModSimPack a **Mod**eling and **Sim**ulation **Pack**age for automatic selection of numerical solvers for a particular simulation problem. ModSimPack takes as input a simulation model expressed in declarative modeling and simulation language such as Modelica. The system is able to detect the types of the equations, perform symbolic manipulations on them and decide which numerical solver is most suitable to solve the problem. ModSimPack also provides an advanced feedback mechanism if inconsistencies and structural singularities are present in the model. The framework gives advices without relying heavily on the user to provide detailed information about the problem to be simulated. The user input is limited to the specification of the model. This is particularly important because most of the users of modeling and simulation systems are not familiar with the requirements of the numerical solvers or with the numerical properties of the simulated system which may affect the choices of different parameters in the solver. ModSimPack emits imperative procedural code that calls the selected numerical solver. The generated code can be compiled and executed by a simulation environment.

The paper will give an overview of the architecture and organization of the framework. In this context, details about the salient features of the equation systems that are exploited by the system to perform the solver selection are given.

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Issues of Model Quality and Validation

SIMULATION MODEL QUALITY ISSUES IN ENGINEERING: A REVIEW

D.J. Murray-Smith

Department of Electronics and Electrical Engineering
University of Glasgow, Glasgow G12 8LT, United Kingdom
Phone:+44 (0)141 330 5222, Fax: +44 (0)141 330 6004
Email: d.murray-smith@elec.gla.ac.uk

Engineering decisions often depend, explicitly or implicitly, on mathematical or computer-based models. Examples of the central role of dynamic models may be found in many application areas, including safety-critical systems. Recent initiatives in the defence and aerospace sector have given new emphasis to the importance of model quality issues (e.g. [1]-[4]).

The design of automatic control systems provides many examples where mathematical models and the associated computer simulations have a particularly important role. Although dynamic models are accepted as being of central importance, relatively little attention has been given to the confidence that can be placed on predictions or the associated design decisions based upon them. Implications for control system design are discussed.

Discussion presented in earlier reviews of model validation and model quality issues (e.g. [5]) is extended and the paper outlines some of the most widely used techniques available for validation of simulation models from tests or measurements made on the corresponding real systems. Recent developments and current trends in this field are discussed and some problems inherent in applying rigorous external validation procedures to complex nonlinear models in integrated system design applications are outlined. Implications for the education and training of engineering students are considered.

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SIMULATION MODEL DEVELOPMENT IN ANALOGY WITH SOFTWARE ENGINEERING

M. Valasek, CTU Prague, Czech Republic

Corresponding Author: M. Valasek
Czech Technical University in Prague
Karlovo nam. 13, 121 35 Praha 2, Czech Republic
Phone: +420 224357361, Fax: + 420 224916709
email: valasek@fsik.cvut.cz

The paper deals with the investigation of the analogy between simulation model development and software engineering. The process of simulation model has been analysed and based on that the life cycle of simulation model development has been described. It enables to investigate the analogy of simulation model development with software development and the possibility to apply and to look for similar procedures of software engineering to the development of simulation models. The paper uses some results of the EU IST 12566 Project CLOCKWORK.

The development of a simulation model and then its simulation typically goes through a number of stages and related tasks. These tasks are illustrated in the life cycle and knowledge framework of simulation model development in Fig. 1. The light arrows represent mappings between the different elements and the black arrows represent transformation processes between the tasks. The development of a simulation, as shown in Fig. 1, involves five steps. It goes from the real world problem through conceptual and physical world into the simulation world split into simulation model implementation and simulation experiments.

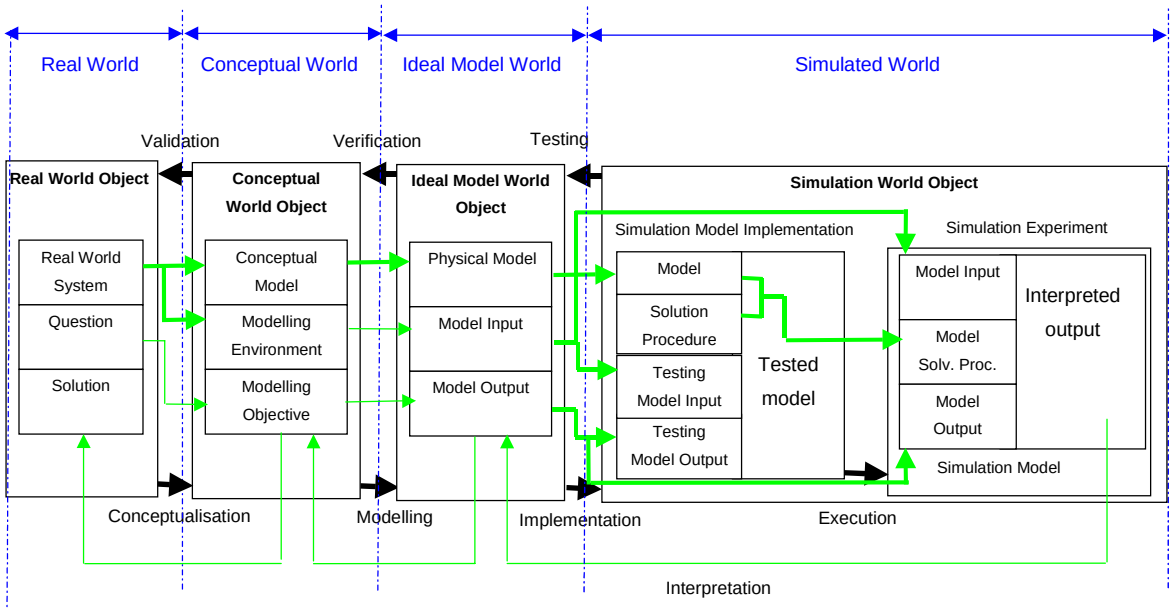

Fig. 1. The Knowledge Framework and Life Cycle of Simulation Model Development

The analyses of the life cycle of simulation model development give direct analogy of simulation model development to the software development. If it is true then many approaches developed in software engineering can be used for simulation model, improvement of their development processes and model qualities. The paper explores initially this topic.

The first analogy between software and simulation model development is the stages of life cycle. The other analogy is between different approaches for software development and currently incomplete approaches for simulation model development. Special attention deserves the inspiration and reuse of techniques for software testing and debugging for simulation model development.

GAUSSIAN PROCESS MODELS VALIDATION: BIOTECHNOLOGICAL SYSTEMS CASE STUDIES

K. Ažman[1] and J. Kocijan[1,2]
[1]Jožef Stefan Institute, Ljubljana, Slovenia
[2]Nova Gorica Polytechnic, Nova Gorica, Slovenia

Corresponding Author: K. Ažman
Jožef Stefan Institute
Jamova 39, SI-1000 Ljubljana, Slovenia
Phone: +386 1 4773 637, Fax: +386 1 4257 009
email: kristjan.azman@ijs.si

The necessary part of every mathematical modelling approach is model validation. Validation is frequently a part of modelling procedure that requires additional computational effort. It might be perceived as a facilitation of the entire modelling process if dynamic system's model simulation results would contain confidence intervals. Gaussian process models appears to be one such model that provides this kind of information. It is a probabilistic, non-parametric, model used mainly in the Bayesian statistics community. With this model the uncertainty associated with the model's prediction is straightforwardly obtained. Despite the current challenges, such as the computational burden associated with the number of training data, the Gaussian process approach has a number of exciting advantages. The simple model structure and the uncertainty information on the predictions are only two of the attractions of the GP approach. Gaussian process models [1] can be used to tackle many of the standard problems usually solved by artificial neural networks and were applied on a range of static nonlinear regression problems. Despite being used mostly to model static non-linearities recently they have been used to model dynamic systems as well, e.g. [2]. Gaussian process (GP) model describes both the dynamic characteristics of nonlinear system, and at the same time provides information about the confidence in its predictions. The model can highlight the areas of the input space where prediction quality is poor due to the lack of data, by indicating the higher variance around the predicted mean.

In this paper we examine the validation of the GP model and show how confidence intervals contribute to information about identified model validity. Two case studies are considered: modelling of activated sludge processes in wastewater treatment plant [3, 4] and modelling of algal growth in the Lagoon of Venice [5, 6]. These two different systems with very different kinds of measurement data sets are used to obtain a model with the purpose of response prediction in a certain time window. Confidence intervals that are inherently part of the obtained models are used as a tool for validation of obtained models on sets of data that were not used for identification and correspondingly interpreted.

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COMPARATIVE EVALUATION OF NONLINEAR IDENTIFICATION APPROACHES

Ch. Märzinger[1], L. del Re, E. Grünbacher, A. Schrempf[2]
Johannes Kepler University Linz, Austria

Corresponding Author: L. del Re,
Johannes Kepler University, Linz
Altenbergerstr. 69, 4040 Linz, Austria
Phone: +43 70 2468-9772, Fax: + 43 70 2468- 9757
email: luigi.delre@jku.at

Abstract. Design of data based models for nonlinear systems using universal approximators has become a standard issue for which several tool boxes exist. The validation of such models is usually done using data of the same range and distribution as the identification data. This fact tends to hide the fact that the choice of the basis function used for the approximation is decisive in terms of model quality, and in particular of its extrapolation qualities. To avoid these problems, this papers analyzes a different class of models, the so called Extended State Affine systems (ESAS), which possess universal approximating properties but are based on expressions likely to occur in real systems. For comparison, the silver box approach was used, i.e. the model quality was valued also for extrapolation.

Before the comparison could be performed, however, robustification was needed for the subspace identification for ESAS, which tends to lead to ill-conditioned problems. Then comparison results were obtained, leading to the clear results:

- Not surprisingly, linear models are superior under several aspects for linear systems, but fail fast for nonlinear ones
- The ratio between model complexity and interpolation quality is not essentially different between the two universal approximator classes, but the essentially non iterative identification procedure for the ESAS will not be consistent if no robustification (e.g. Tychonov) is used
- The picture changes completely once the extrapolation properties are considered. In this case, clear advantages of the ESAS models are found.

The tests have been performed, among others, on data of a test bench structure, for which both a real plant and a good, physical model are available. The following table summarizes the results of two ESAS versions, a linear model and artificial neural networks for the extrapolation: the degradation of the performance of ANN compared to ESAS is evident. The paper gives an explanation of these effects in terms of properties of the approximating functions implied in the ESA and in the ANN.

2*VAF	Interpolation	Extrapolation
ESA-TR	1.96944	1.9651
ESA-TTLS	1.97102	1.9671
ARMAX	1.88723	1.9019
ANN	1.92031	1.4305

Table. 1: Scaled VAF values for SNR 30dB

[1] Present address: BMW Motoren Steyr, Austria
[2] Present address: FH für Merdizinaltechnik, Linz

FAULT DETECTION BASED ON GAUSSIAN PROCESS MODELS

D. Juričić[1] and J. Kocijan[1,2]
[1]Jozef Stefan Institute, Ljubljana, Slovenia
[2]Nova Gorica Polytechnic, Nova Gorica, Slovenia

Corresponding Author: D. Juričić
Jozef Stefan Institute
Jamova 39, SI-1000 Ljubljana, Slovenia
Phone: +386 1 4773 661, Fax: +386 1 4257 009
email: dani.juricic@ijs.si

Model validation has been considered as a well established discipline particularly in what regards control design and prediction. Surprisingly, little attention has been paid so far to validation issues in cases when model is intended for fault detection and isolation. Indeed, typical model quality assessment in such cases reduces to model falsification through comparing measured and simulated output signals and testing residuals with respect to various statistical properties. However, it has been often overlooked, especially in nonlinear systems diagnosis, that model precision, achieved on a learning set Γ_l and possibly validated on a set Γ_v is not necessarily the same across the complementary set $\Gamma_c = \overline{\Gamma_l \cup \Gamma_v}$. The problem we address is how to preclude false and missed alarms in cases when the model-based detector operates on data from Γ_c.

In this paper we try to show that detection problems encountered in under-modelled operating modes can be consistently treated by a novel modelling approach referred to as Gaussian Process (GP) Model, used in the Bayesian statistics community. With this model we straightforwardly obtain the predictive uncertainty associated with the model response, which is in general difficult to evaluate appropriately with nonlinear parametric models, where model prediction and predictive uncertainty are dealt as separate issues.

In the paper, the problem of a trade-off between robustness towards errors caused by invalidated models and sensitivity to faults is put into a statistical framework. We restrict in this paper on sensor faults. The main idea is to exploit the information about the prediction uncertainty, which is inherently present in the Gaussian process model, for estimating the confidence into detection rules. One of the contributions of this paper concerns a validity index that provides such an estimation. Another contribution regards a likelihood ratio test derived for Gaussian Process models, which reduces to checking whether a weighted sum of residuals exceeds some predefined threshold.

The ideas related to dynamic modelling and detection rule synthesis are illustrated on a simulated pH process.

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KNOWLEDGE SUPPORT OF SIMULATION MODEL DEVELOPMENT BY REUSE

M. Valasek, P. Steinbauer, Z. Sika, CTU Prague, Czech Republic
Z. Zdrahal, P. Mulholland, Open University Milton Keynes, UK

Corresponding Author: M. Valasek
Czech Technical University in Prague
Karlovo nam. 13, 121 35 Praha 2, Czech Republic
Phone: +420 224357361, Fax: + 420 224916709
email: valasek@fsik.cvut.cz

The paper deals with the knowledge framework of simulation model development and based on it with the methodology, techniques, procedures and software for knowledge support of simulation model development by reuse. The paper is based on the results of the EU IST 12566 Project CLOCKWORK.

The simulation of dynamic systems is in nature a knowledge intensive activity, but analysing the resulting documentation of such activities shows that there is a significant loss of knowledge, creating problems for team communication and future reuse. The resulting simulation models do not include the majority of knowledge which was necessary for their development.

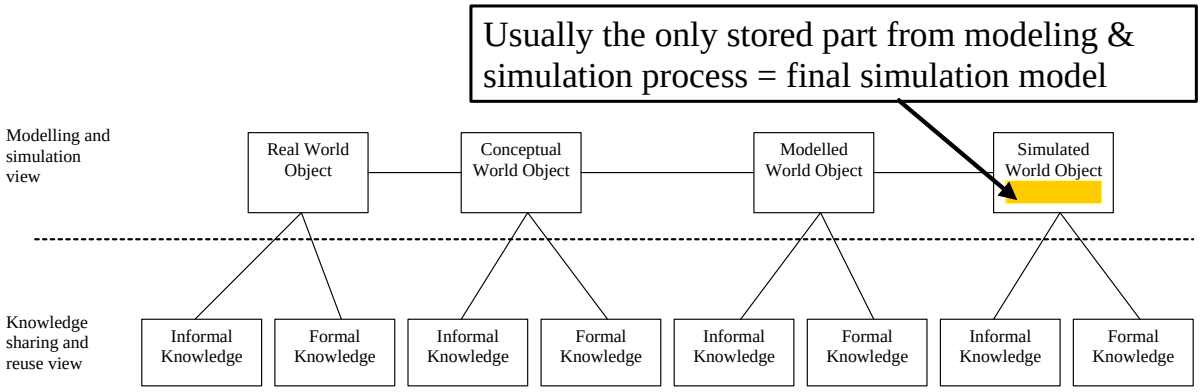

Fig. 1 Development process and different knowledge of simulation model

The development of a simulation model and then its simulation typically goes through a number of stages and related tasks (Fig. 1). It involves five steps. It goes from the real world problem through conceptual and physical world into the simulation world split into simulation model implementation and simulation experiments. The development produces a large amount of knowledge. This knowledge is of two kinds – informal and formal. Informal knowledge takes the form of text and diagrams, typical for different engineering models and schemes, often also called informal annotations. Formal knowledge describes the models and associated processes according to concepts represented in an ontology. An ontology is an explicit conceptualisation of a domain. The ontology therefore contains concepts applicable across some domain such as the simulation and modelling of mechatronic machinery. The associations between the ontology and specific simulation models are specific for each case and provided by so called semantic indexes.

Based on this knowledge framework a set of techniques, procedures and software tools for capture, storage and retrieval of knowledge used and accumulated during simulation model development have been developed. The reuse of stored cases of simulation models and their development processes is based on the retrieval of similar cases from knowledge database using the captured knowledge and its repeated understanding and interpretation. This approach towards simulation model reuse based on knowledge support contributes significantly to the issues of model quality and model validation.

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Model Reduction and Reduced Order Modelling

Parameter Preserving Model Reduction for MEMS System-level Simulation and Design

E. B. Rudnyi, C. Moosmann, A. Greiner, T. Bechtold, J. G. Korvink
IMTEK, Freiburg University, Germany

Corresponding Author: J. G. Korvink
Lab of Simulation, Department of Microsystems Engineering (IMTEK), University of Freiburg
Georges-Köhler-Allee 102 00 086, 79110 Freiburg, Germany
Phone: +49 761 203 7436, Fax: +49 761 203 7437
email: korvink@imtek.uni-freiburg.de

The microelectronic industry enjoys tremendous productivity levels due to its high level of design automation (EDA). This is possible because the industry has agreed on how design should progress, and what the future priorities are in terms of necessary achievements. In microsystem and nanosystem development this has not yet happened [1], mainly because the industry is not yet mature enough, but especially because the microsystem design automation industry is in its infancy.

Model order reduction is a rapidly developing interdisciplinary area (see, for example [2][3]). There is considerable progress in the application of modern model reduction to MST for the last five years and, in our opinion, model reduction has great potential to automatically develop compact models needed for microsystem design automation.

However, conventional model reduction fails to preserve parameters during model reduction process. This limits severely its applicability for the design flow and system-level simulation. In the present paper we demonstrate how one can overcome this limit by means of multivariate expansion [4].

We report the results of multivariate moment matching for several MEMS models:

- Device cooled by airflow: preserving a film coefficient;
- Flow meter (anemometer): preserving the flow velocity;
- Microelectrode: preserving the applied voltage.

We demonstrate that the method allows us to build an accurate low-dimensional model that precisely captures dynamics of the original model in a wide parameter range.

We also discuss how to automatically choose moments to include into the reduced model. A straightforward approach which generates all the moments up to a given order does not scale well with the number of parameters [4]. For example, if we choose to preserve four parameters then a reduced model made from all first derivatives has the dimension of 6, a reduced model made from all second derivatives has the dimension of 21, and a reduced model from all third derivatives already has the dimension of 56 (see Appendix F in [4]). At the same time, we may need derivatives of higher order than three to describe accurately the transient behavior of the original model.

In order to treat the problem, we suggest a heuristic procedure. It is based on 1) neglecting the mixed moments; 2) employing local error control to chose the right number of moments along the Laplace variable and each parameter. We apply it for the first device in the list above to preserve three film coefficients independently and report results.

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MULTI-PARAMETER POLYNOMIAL MODEL REDUCTION OF LINEAR FINITE ELEMENT EQUATION SYSTEMS

O. Farle, V. Hill, P. Ingelström, and R. Dyczij-Edlinger, Saarland University, Germany

Corresponding Author: O. Farle,
Lehrstuhl für Theoretische Elektrotechnik, Saarland University
Building C63, P. O. Box 151150, D-66041 Saarbrücken, Germany
Phone: +49 681 / 302 -3194, Fax: +49 681 / 302 -3157
email: o.farle@lte.uni-saarland.de

In this paper we present a new method for the model order reduction of linear equations systems parameterized by polynomials in several variables, $s_1 \ldots s_K$. The considered equation systems take the form

$$\left(\sum_{m_1+\ldots+m_K<M} s_1^{m_1} \ldots s_K^{m_K} \mathbf{M}_{m_1 \ldots m_K} \right) \mathbf{x} = \sum_{m_1+\ldots+m_K<M} s_1^{m_1} \ldots s_K^{m_K} \mathbf{b}_{m_1 \ldots m_K} \tag{1}$$

and stem from the finite element simulation of passive microwave systems. Typical parameters include the operating frequency and material properties.

The proposed method is a projection-based approach using Krylov subspaces [1][2] and extends the works of [3][4]. First, we present the multivariate Krylov space of higher degree associated with a parameter-dependent right-hand-side vector and derive a general recursion for generating its basis. Next, we propose an advanced algorithm to compute such basis in a numerically stable way. Finally, we apply the Krylov basis to construct a reduced order model of the moment-matching type. The resulting single-point method requires one matrix factorization only.

In the presentation, we shall develop the underlying theory and give numerical examples to demonstrate the efficiency and reliability of the proposed approach.

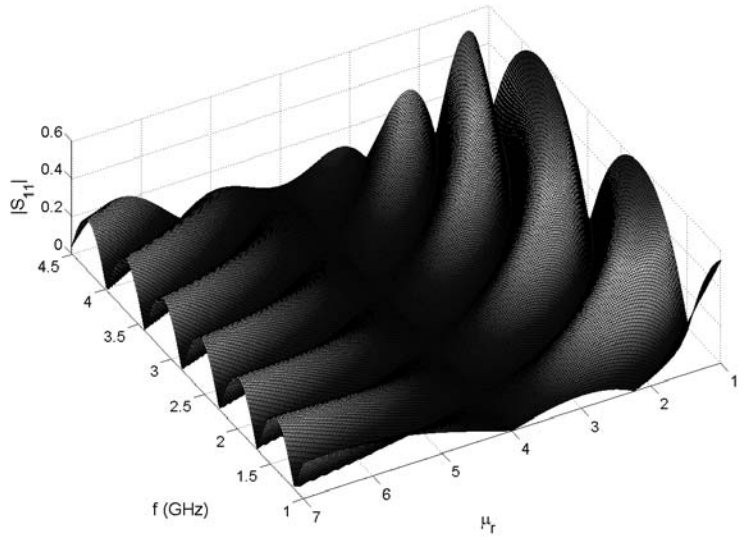

Fig. 1. Magnitude of reflection coefficient of microwave structure as a function of frequency and magnetic permeability

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CONTROLLER REDUCTION: AN OBSERVER BASED APPROACH

A. Yousefi and B. Lohmann, TU Munich, Germany

Corresponding Author: A. Yousefi
Technical University of Munich
Boltzmann Str. 15, D-85748 Garching, Germany
Phone: +49 89 289-15670, Fax: + 49 89 289-15653
email: Yousefi@tum.de

In this work a reduced order controller design approach based on Linear Quadratic Regulators, in order to improve the simplicity and reduce the online computation effort is studied. The use of an optimization method allows the simultaneous tuning a controller, seeking a trade-off between the different performance objectives and exploiting a controller reduction method prevents from arising of sampling interval limits. We have merged these two approaches by taking advantage of the idea of reduced observers into a new method for designing low order controller for high order plants.

The reasons that simple controllers are normally preferred over complex ones are trivial. It is clear that when we are dealing with low order controllers, there are fewer things to go wrong in the hardware or bugs to fix in the software; they are easier to understand and the computational requirements are less. In order to achieve these advantages, there are lots of efforts to invent new methods which yield low order controllers in comparison to the typical ones. In [1] such methods are divided into two classes: direct and indirect. In direct methods the parameters defining the low order controllers are evaluated by some predefined procedure, while in indirect methods at first a high order controller is found and then a procedure (like weighted approximation [2]) is used to simplify it. Our method in this paper is mostly focused on the linear quadratic regulators (LQR), which means the controller design consists of an observer and a state feedback gain. Therefore this approach is more likely categorized in the second class of reduced controller methods (indirect). Our choice of LQR is based on its outstanding properties and its popularity among control engineers. It is well known that the LQR design technique has been developed to produce stable multi-input multi-output (MIMO) systems with good performance characteristics [3].

The goal is to design a strictly proper controller of lower order with similar structure to LQR (observer plus state feedback) such that it satisfies the following design criteria:

- The observer part be a steady state asymptotic observer for a specified dimensional subspace of the plant.
- The controller (the observer with accompanying a constant gain matrix Kr) be a stabilizing compensator.

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BALANCED TRUNCATION MODEL REDUCTION OF SECOND-ORDER SYSTEMS

Tatjana Stykel, TU Berlin, Germany

Institut für Mathematik, MA 3-3
Technische Universität Berlin
Straße des 17. Juni 136
10623 Berlin, Germany
Phone: +49 30 314-29292, Fax: +49 30 314-29621
email: stykel@math.tu-berlin.de

Consider a linear time-invariant second-order system

$$\begin{aligned} M\,\ddot{q}(t) + D\,\dot{q}(t) + K\,q(t) &= B_2 u(t), \\ C_2\dot{q}(t) + C_1 q(t) &= y(t), \end{aligned} \tag{1}$$

where $M \in \mathbb{R}^{n,n}$ is a mass matrix, $D \in \mathbb{R}^{n,n}$ is a damping matrix, $K \in \mathbb{R}^{n,n}$ is a stiffness matrix, $B_2 \in \mathbb{R}^{n,m}$, C_1, $C_2 \in \mathbb{R}^{p,n}$, $q(t) \in \mathbb{R}^n$ is a displacement vector, $u(t) \in \mathbb{R}^m$ is a control input and $y(t) \in \mathbb{R}^p$ is an output vector. Such large-scale systems arise frequently in many practical applications including electrical circuit simulation, structural dynamics and micro-electro-mechanical systems. The model reduction problem consists in an approximation of system (1) by a low-dimensional model

$$\begin{aligned} \widetilde{M}\,\ddot{\widetilde{q}}\,(t) + \widetilde{D}\,\dot{\widetilde{q}}\,(t) + \widetilde{K}\,\widetilde{q}(t) &= \widetilde{B}_2 u(t), \\ \widetilde{C}_2\dot{\widetilde{q}}\,(t) + \widetilde{C}_1\widetilde{q}(t) &= \widetilde{y}(t), \end{aligned} \tag{2}$$

where $\widetilde{M}$, $\widetilde{D}$, $\widetilde{K} \in \mathbb{R}^{\ell,\ell}$, $\widetilde{B}_2 \in \mathbb{R}^{\ell,m}$ and $\widetilde{C}_1$, $\widetilde{C}_2 \in \mathbb{R}^{p,\ell}$ with $\ell \ll n$. We require for the approximate system (2) to be stable and passive if (1) is stable and passive and to have a small approximation error.

A common approach for reducing the dimension n of (1) is to rewrite this system as an equivalent first-order system of the state space dimension $2n$ and then to apply any known model reduction method. A drawback of this approach is that the reduced first-order system cannot, in general, be represented in the second-order form (2). Note that the preservation of the second-order structure in the reduced systems is important for physical interpretation.

In this talk we will discuss recent progress and some challenges in structure-preserving model reduction of second-order systems. In particular, we will focus on a balanced truncation method which has been proved to be an efficient model reduction method for first-order large-scale systems. This method is based on a state space transformation of the dynamical system into a balanced form whose controllability and observability Gramians are equal and diagonal, together with a truncation of those states that are irrelevant in some sense. Important properties of the balanced truncation method for the first-order systems are that the stability is preserved in the reduced system and there is a priori error bound.

For system (1), two pairs of Gramians have been introduced in [1, 2]. These are the position controllability and observability Gramians $\mathcal{P}_p$ and $\mathcal{Q}_p$ and the velocity controllability and observability Gramians $\mathcal{P}_v$ and $\mathcal{Q}_v$. They are defined as diagonal blocks of the controllability and observability Gramians

$$\mathcal{P} = \begin{bmatrix} \mathcal{P}_p & \mathcal{P}_{12} \\ \mathcal{P}_{21} & \mathcal{P}_v \end{bmatrix}, \qquad \mathcal{Q} = \begin{bmatrix} \mathcal{Q}_p & \mathcal{Q}_{12} \\ \mathcal{Q}_{21} & \mathcal{Q}_v \end{bmatrix}$$

of the corresponding first-order system. Using the position and velocity Gramians we can define different concepts of balanced realizations and singular values for the second-order system (1). The latter play a crucial role in identifying which states are important and which states can be truncated without changing the system properties significantly. We will compare different variants of second-order balanced truncation on numerical examples.

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PASSIVE REDUCED ORDER MODELLING OF SECOND ORDER SYSTEMS BY BACK CONVERSION

B. Salimbahrami and B. Lohmann, TU Munich, Germany
A. Bunse-Gerstner, University of Bremen, Germany

Corresponding Author: B. Salimbahrami
Technical University of Munich
Boltzmann Str. 15, D-85748 Garching bei München, Germany
Phone: +49 89 289-15659, Fax: + 49 89 289-15653
email: salimbahrami@tum.de

In some fields like electrical and mechanical engineering, modelling (for instance by FEM) leads to a large number of *second* order differential equations. In order reduction of such systems, it is advisable to approximate the behaviour of the original systems while preserving the structure, stability and passivity.

As numerical cost and reliability are of great importance in order reduction of large scale systems, methods like moment matching using Krylov subspaces are usually favorable. A generalization of Krylov subspace methods which preserves the second order structure can be found in some recent works. A passivity preserving method for second order systems called Structure-Preserving Reduced-Order Interconnect Macromodeling (SPRIM) has been introduced by Roland Freund that preserves the structure and passivity of the original system. This method considers the equivalent state space model and a projection with a special structure is applied to the system such that the structure of the state space matrices is preserved. The disadvantages of SPRIM are matching smaller number of moments compared to the standard Krylov subspace methods and there are some difficulties in matching the moments around zero as a column of the projection matrix becomes zero.

The high-order models considered in this paper are assumed to be given in the form,

$$\begin{cases} \mathbf{M}\ddot{\mathbf{z}} + \mathbf{D}\dot{\mathbf{z}} + \mathbf{K}\mathbf{z} = \mathbf{G}\mathbf{u}, \\ \mathbf{y} = \mathbf{L}\dot{\mathbf{z}}. \end{cases} \tag{1}$$

In this paper, two different methods are proposed. The first approach is based on a direct projection using a Second Order Krylov Subspace method matching up to $q+1$ moments of the original and reduced systems, where $Q = 2q$ is the order of the reduced system in SISO case. For a passivity preserving reduction, the sufficient conditions $\mathbf{D} + \mathbf{D}^T \succeq 0$, $\mathbf{K} = \mathbf{K}^T \succeq 0$, $\mathbf{M} = \mathbf{M}^T \succeq 0$ and $\mathbf{L} = \mathbf{G}^T$ should be satisfied. The advantage of applying the projection directly to the second order system are that some properties of the original matrices (e.g. symmetry, positive-definiteness, diagonality) are preserved and an undamped model results in an undamped reduced system. However, smaller number of moments match compared to the state space approaches.

In the second method, the number of matching parameters is increased by reducing the equivalent state space model and then recovering the second order structure by applying a similarity transformation to the reduced system. For the reduction step a one-sided method Krylov subspace method is used, matching $Q = 2q$ moments. The passivity is preserved if the sufficient conditions $\mathbf{A} + \mathbf{A}^T \preceq 0$, $\mathbf{E} = \mathbf{E}^T \succeq 0$ and $\mathbf{C} = \mathbf{B}^T$ are satisfied. A structural property of the original system is that the first moment around zero is zero that should be preserved in the reduced system through moment matching.

To match the moments around s_0, the cost of calculation can be reduced up to 8 times by explicitly calculating the matrix inverse involved in the Krylov subspace. An algorithm is proposed to reduce second order systems while considering the structure of the matrices where only the inverse of the matrices $\mathbf{K}$ and $\mathbf{K}_0 = s_0^2\mathbf{M} + s_0\mathbf{D} + \mathbf{K}$ are to be calculated instead of inverse of $\mathbf{A}$ and $\mathbf{A} - s_0\mathbf{E}$ of double dimension.

An additional condition compared to the first approach is that the stiffness matrix $\mathbf{K}$ should be nonsingular and the numerical algorithm is more expensive as it needs twice the number of iterations to reduce to the same order. However, the back conversion method matches almost twice the number of moments leading to a better approximation. This is also confirmed by the example in the paper.

Compared to SPRIM, in both methods, the projection matrix is always full rank and the difficulty to match the moments around zero is solved. As an example, we apply different methods to an RLC network with application in modelling of transmission lines. The results show the superiority of the back conversion method compared to others.

ORDER REDUCTION OF FIRST AND SECOND ORDER SYSTEMS USING LAGUERRE SERIES AND MOMENT MATCHING

R. Eid, B. Salimbahrami and B. Lohmann, TU Munich, Germany

Corresponding Author: R. Eid
Technical University of Munich
Boltzmann Str. 15, D-85748 Garching, Germany
Phone: +49 89 289-15681, Fax: + 49 89 289-15653
email: eid@tum.de

In our rapidly developing technological world, complex and large scale first and second order systems are becoming more and more encountered with an increasing application in control Engineering, circuit simulation, micro-electro-mechanical systems (MEMS), microelectronics (VLSI) design, aerospace and civil engineering etc. As it is very difficult to handle these systems by current digital computers due to memory, ac-curacy or executing time problems, it is advisable to calculate a reduced order model that approximates the behavior of the original system in order to simplify the tasks of simulation, controller design, optimization and prediction.

The reduction methods based on matching the moments and/or Markov parameters of the original and reduced models using the Krylov subspaces are nowadays among the best choices [1]. The moments are the coefficients of the Taylor series expansion of the transfer function around a certain point and if the Taylor series expansion around infinity is considered the coefficients are called Markov parameters. These methods find the reduced order model in a relatively short time with a good numerical accuracy, via a projection whose columns form bases of particular Krylov subspaces.

Lately, the idea of order reduction was coupled to different orthonormal series (Laguerre, Legendre, ...) as an alternative to the Taylor series. Instead of moment matching, these alternative approaches match some of the coefficients of the chosen series of the reduced and original models' transfer functions.

In this paper, the order reduction of first order systems using Laguerre series expansion is reviewed [2] and then this approach is generalized to reduce second order systems while preserving the structure, by introducing two different methods based on the Krylov subspaces. In addition, the connection between the classical moment match-ing approach and the Laguerre-based reduction approach is investigated and the equivalence between those two methods under specific conditions is proved.

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A SPECIAL METHOD FOR CONTROLLER REDUCTION

A. Hofer

Institute of Automation and Control, Graz University of Technology
Inffeldgasse 16c, 8010 Graz, Austria
Phone: +43 316 873 7022, Fax: +43 316 873 7028
email: Anton.Hofer@TUGraz.at

In this paper a controller reduction method is presented, which is tailored to the specific situation in the so-called Q-design framework [1] for linear control systems. Generally there is a fundamental difference between the common problem of model reduction and the problem of controller reduction. This is caused by the fact that the primary goal is not a good approximation of the behaviour of a given high order controller by a low order one. On the contrary, the main focus is *to maintain the performance of the closed loop control system* when the high order controller is replaced by a low order controller. Therefore many of the well known methods for model reduction cannot be applied to controller reduction problems directly. In many cases the methods have to be modified or new approaches for controller reduction have to be established. Actually there are controller reduction methods available which are based on frequency weighted H_∞-techniques, frequency weighted reduction in the state space, reduction schemes based on coprime factorization or partial fraction expansions. A comprehensive overview of all these approaches is given in [3].

It is a severe disadvantage of the Q-design design method that the resulting controllers often suffer from inflating order. This is especially the case if this procedure is applied to MIMO systems and the l_1-norm [2] is used to formulate the design goals. Since the result of the design procedure in the l_1-case is given by the truncated impulse responses of some closed loop transfer matrices none of the known controller reduction methods can be applied directly. Furthermore we are in the remarkable situation that due to possible numerical problems the mathematical model of the high order controller should not be used during the reduction process. Taking into account this specific requirement, a method for controller reduction is developed. It is a characteristic feature of the proposed strategy that the task of controller reduction is translated into a convex optimization problem especially into a linear program. In doing so an LTI controller of low order is computed such that the frequency response of the closed loop transfer matrix (with the high order controller) is approximated as good as possible. For this purpose a suitable frequency discretization has to be selected and based on that a measure for the approximation error is introduced. Now the coefficients of the denominator and numerator polynomials of the low order controller transfer matrix are determined such that the approximation error takes its minimum value.

The proposed method has the drawback that the stability of the closed loop system with the low order controller can only be checked after the reduction process has been performed. This is caused by the fact that all necessary and sufficient stability conditions are non-convex in the chosen controller parameters. Therefore these conditions cannot be incorporated into the linear program for controller reduction on principle. Only in the SISO case some simple sufficient conditions for stability are available which can be formulated as linear inequalities and thus can be easily included to the linear program. However in many examples these sufficient conditions have been proven to be by far to conservative for the controller reduction. The application of the proposed controller reduction method is demonstrated by two examples. In both cases the performance of the reduction method is checked by comparisons of the behaviour of the closed loop systems with the high and the low order controller in the time domain and in the frequency domain.

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Mechanical Systems

MODELLING THE AIR PATH SYSTEM OF DIESEL ENGINES BY QUASI-LPV IDENTIFICATION TECHNIQUES

Xiukun Wei, Luigi Del Re, Univ. Linz , Austria

Corresponding Author: Xiukun Wei
Johannes Kepler University of Linz
Altenberger Straße 69, A-4040 Linz, Austria
Phone: +43 1 732-24689767, Fax: + 43 1 732-24689759
email: wei.xiukun@jku.at

Control oriented air path modelling has been studied for many years. An early mean value model can be found in [1] where the diesel engine modelling procedure based on the first principle is discussed. The modelling and control issues in turbo charged diesel models equipped with variable geometry turbine and exhaust gas recirculation system are reported in [2]. In [3] the multi-variable control of air path systems is considered by different control approaches respectively, and satisfying progress is achieved. This paper has the same goal to get a dynamical model for air path systems of diesel engines; however, the main technique used here is the quasi-LPV system identification. The modelling procedure is divided into three steps. In the first place, a model from exhaust manifold pressure to boost pressure is identified where the exhaust manifold pressure is adopted as the input. Secondly, the exhaust manifold pressure is modelled where the variable geometry turbine (VGT) vane position, fuel mass flow and the product of boost pressure and engine speed are selected as the inputs. The air mass flow model is identified in the last step. As a result, the final model of the system is the combination of the three models. It turns out that the final simplified model of the air path system is a quasi-LPV model with nonlinear static inputs shown in Fig. 1.

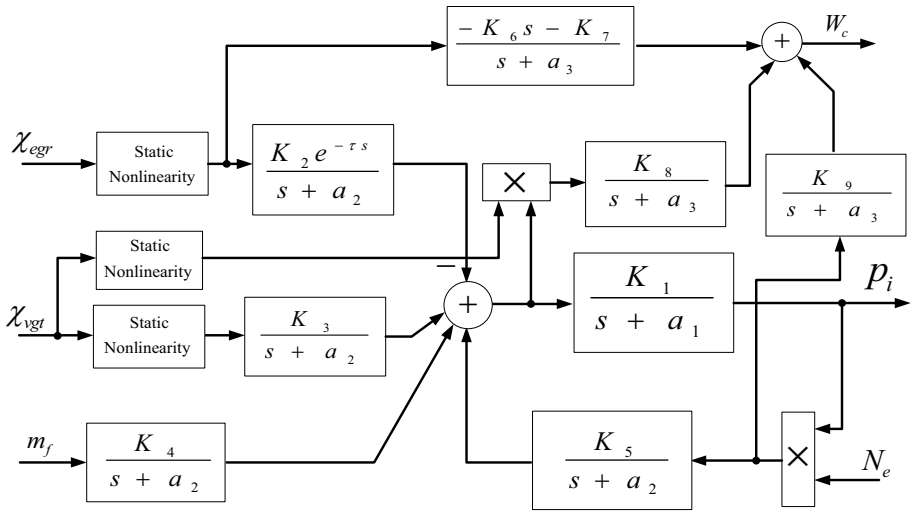

Figure 1. The air path model for a BMW M47 diesel engine

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MODELLING OF THE AIR-SYSTEM OF A TWO-STAGE TURBOCHARGED PASSENGER CAR DIESEL ENGINE

D. Schwarzmann, R. Nitsche, Robert Bosch GmbH, Germany
and J. Lunze, Ruhr-Universität Bochum, Germany

Corresponding Author: D. Schwarzmann
Corporate Sector Research and Advance Engineering of Robert Bosch GmbH
Robert–Bosch–Strasse 2, 71701 Schwieberdingen, Germany
Phone: +49 711 811 – 49448
email: dieter.schwarzmann@de.bosch.com

Today, virtually all modern passenger cars with diesel engines are turbocharged using a single turbocharger. However, tight and diametrically opposed demands concerning better performance, better exhaust quality and higher mileage require new solutions for modern direct injection diesel engines. In order to overcome known problems of turbocharged engines like turbo lag and boost threshold, current research is going towards the usage of various combinations of turbochargers. An example is the two-stage turbocharged diesel engine shown in Figure 1, which is the motivation for this work.

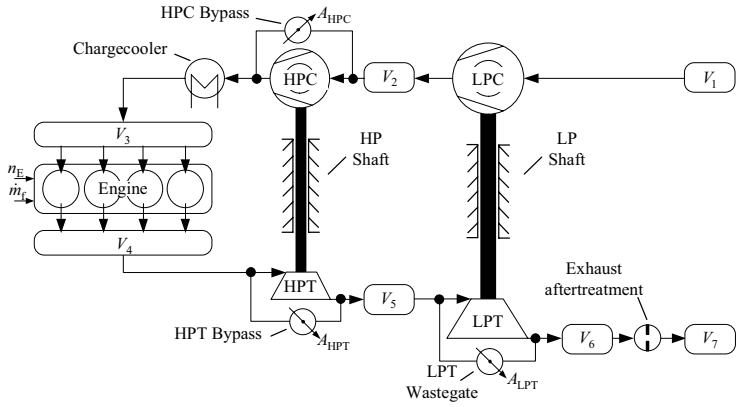

Figure 1: Air-system of a two-stage turbocharged Diesel engine showing the flow of air and exhaust

This paper presents a modular approach of modelling turbocharged diesel engines, focusing on control-oriented models. This means, that component models are presented whose appropriate connection leads to the desired overall model. To this end, a connection method is presented which defines physically meaningful in- and output signals of the components. The component models are divided into two types, namely storage models and coupling models. Figure 2 exemplifies the connection method by a model of an equalisation procedure. All components used to model the system in Figure 1 are described individually. All component models except for turbine and compressor are derived from thermodynamic and mechanical laws. The component models of turbine and compressor have a physical framework, however, their mass flow and efficiency is modelled by a novel parameterised extrapolation of measurement data.

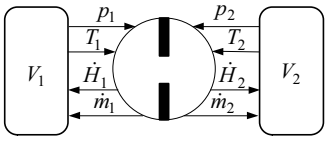

Figure 2: Example of the connection method: Equalisation procedure between two tanks

To the knowledge of the authors, no control-oriented low-frequency model of a two-stage turbocharged diesel engine has been published yet. When compared to other models of single stage turbocharged engines, there are two major contributions of this paper. First, the component driven approach which enables to model many other configurations beside the one shown in Figure 1. Second, the novel extrapolation procedure of measurement data for turbines and compressors.

The final model of the air-system of a two-stage turbocharged diesel engine has twelve states and can be used for control design. A simulation of the model is compared to measurements of an engine test stand and shows excellent accuracy.

A LINEAR PARAMETRIC MODEL OF AN AIR-CONDITIONING UNIT WITH OPERATING POINT DEPENDENT PARAMETERS UNDER NEARLY STEADY WEATHER CONDITIONS

Tawegoum [1] R., Lecointre [2] B.

Corresponding author: R. Tawegoum
[1] Unité de Sciences Agronomiques appliquées à l'Horticulture SAGAH A_462, Institut National d'Horticulture, 2, rue Le Nôtre 49045 Angers, France;
Phone: + 33. (0)2.41.22.54.53; Fax: +33 (0)2.41.22.55.53
[2] Ecole Supérieure des Sciences Appliquées pour l'Ingénieur de Mulhouse, 12, rue des Frères Lumière 68093, Mulhouse, France.
E-mail: tawegoum@angers.inra.fr

Abstract

This paper deals with the identification and the stability analysis of the dynamic models of an air-conditioning unit for growth chambers, a unit that is passive and does not use the more typical compression system or absorption-refrigeration cycle. Growth chambers are useful in the study of plant development and particularly to understand the physical and biological mechanisms involved in the interaction between relative humidity changes and the morphological responses of the plant (growth stoppage, floral transformation, delayed blossom-time, dormancy, etc.).

The unit is composed of two flows: a non-saturated flow and a saturated flow, in the saturated air flow, fresh air is saturated in corrugated pads after being heated by a resistor coil. In the unsaturated air flow, fresh air is only heated by another resistor coil. The specificity of the system is to produce a variable microclimate with variable temperatures and constant moisture set-point values. Since the air-conditioning unit principle is based on the mixing of two types of air, the mixing proportion will change with the temperature and humidity set-points. Due to the changes in operating conditions, the system needs to be modelled using model-based control techniques, despite the fact that it is a model based on physical laws. The problem addressed in this paper is the identification of a multi-input/multi-output model that takes the main dynamic features of the plant into account, provided that the identified model is reasonably usable with conventional linear control approach and is covered the experimental set of data.

The system is a MIMO with two uncontrollable inputs, the air inlet and the water flowing through the pads. The other inputs are the voltages applied on the heaters, and the voltage on the DC motor. Air temperature after the pads, and the relative humidity downstream of the dry pads were the output variables. A preliminary analysis of the steady state gain and the time constant of different outputs of the air-conditioning unit showed that their values varied with regard to the aperture position. The process had a linear representation around each operating point.

Experiments were performed to identify the structure and coefficients of the model around the main operating points. Using the Linear Model Operating Dependent Parameter, the models were parameterised using polynomial functions in order to provide a single structure for the system. The ARMAX (2 3 2 1) model obtained for the temperature in the saturated flow was as follows: $A(q,\zeta(t)).y(t) = B(q,\zeta(t)).u(t-k) + C(q,\zeta(t)).e(t)$. The ARX (2 2 1) model obtained for the temperature and the relative humidity in the non-saturated flow was as follows: $A(q,\zeta(t)).y(t) = B(q,\zeta(t)).u(t-k) + e(t)$. The coefficients were three-degree polynomials, depending on ζ,In the saturated flow, the best fit prediction was around 80%, and in the non-saturated flow, the mean of the best fit varied around 85% for temperature and around 65% for relative humidity. The results show that the predictions are very close to the measurements, except for the relative humidity, due probably to a partial deshumidification though dry pads.

The open loop stability conditions were derived from a reduced free model. We verified that closed loop stability was maintained using a class of feedback controls.

The model predicts system behaviour provided that the external parameters have low variations of amplitude. To make it applicable to a broader range of conditions, the characteristics of the inlet air and water pad variability must be taken into account. In order to do this, recursive identification and direct non-linear identification are presently being studied.

MATHEMATICAL MODELING OF DYNAMIC PROCESSES OF BUCKET WHEEL EXCAVATORS

Srdjan Bosnjak, Zoran Petkovic, Nenad Zrnic, Slobodan Petric

Corresponding Author: S. Bosnjak,
University of Belgrade, Faculty of Mechanical Engineering
Kraljice Marije 16, 11000 Belgrade, Serbia & Montenegro
Phone: +381 11 3302–290, Fax: + 381 11 3370–364
Email: sbosnjak@mas.bg.ac.yu

Bucket wheel excavators (BWE) belong to the class of machinery with significant dynamic loadings having stochastic character. To go through the comprehensive analysis of their dynamic behavior, having in mind the possibility of resonant states occurrence, it is necessary to create suitable machine dynamic model as well as a model for excitation due to the resistance of excavation. This paper discusses procedures for creating reduced dynamic models of dominant substructures of BWE. Models shown in this paper have spatial character and they enable possibility of coupling with excitation model, figure 1. The procedure of excitation identification (resistance to excavation) takes into account all structural and machine's duty cycle parameters. Stochastic effect of resistance to excavation is simulated by random numbers generator. This paper estimates the rheolineral level of mathematical model and possibility of structural parametric vibrations occurrence for BWE KRUPP 1760.

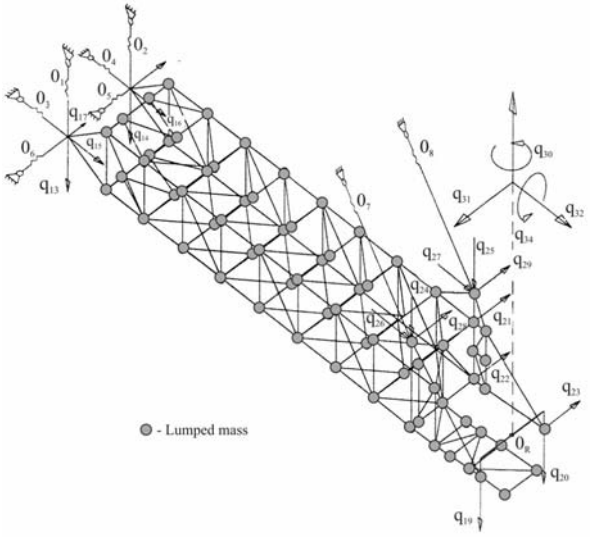

Figure 1: Reduced spatial dynamic model of bucket wheel boom

Moreover, this paper presents dynamic behavior analysis for reducer in the drive for bucket wheel boom lifting for BWE TAKRAF SRs 1200. It is observed that non–synchronized operation of driving motors as well as operation of braking system can cause malfunction of the flexible coupling in input reducer shaft. In order to correct these effects reducer output shaft and connecting shaft are connected with rubber elastic coupling. Based on the response of dynamic model of reducer, it is conclusive that the amplitude of changing torque for output shaft is smaller for mechanism with built in rubber flexible coupling, as a consequence of amortization of higher vibrations modes of excitation force. The validation of procedure for modeling external loadings of bucket wheel, and thereby for the reducer of observed system, was done based on measurements in real operating conditions. Analysis of dynamic behavior of the BWE presented in this paper ensures a more complete definition of the machine performance and helps to perceive its effects upon the design of particular units and subsystems.

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MODELLING AND ANALYSIS OF MACHINE TOOLS AND CONVERTING MACHINES

E. Schäfers, Siemens AG, Germany

Siemens AG A&D MC RD 2
Motion Control Systems
Frauenauracher Str. 80, 91056 Erlangen, Germany
Phone: +49 9131 98 3301, Fax: + 49 9131 98 2596
Email: elmar.schaefers@siemens.com

To develop machines, which fulfil today's requirements regarding machine dynamics, it is necessary to optimize the complete mechatronic system with respect to dynamic aspects. This contribution will focus on the area of generating suitable models for machine tools and converting machines.

First, basic structures of lumped mass models are derived which cover restricting machine features. These models can be used to interpret frequency domain measurements and allow allocating weak points of a construction. Figure 1 shows an example of a machine axis model including both the influence of the machine base and the stiffness loss caused by the ball screw system.

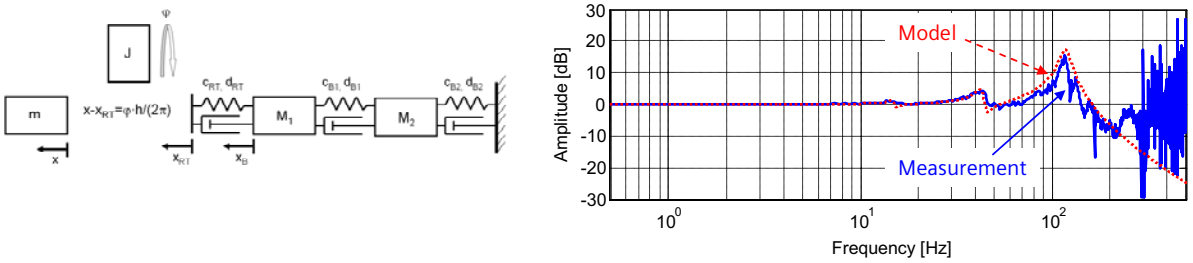

Figure 1: Left: Model of the mechanics of a machine axis, right: Measured and simulated amplitude of the frequency response, (velocity of table relative to machine base) / (motor speed).

Next, to get a better insight into the behaviour of a complete mechatronic system, a simplified way to integrate the influence of PI-control parameters into the model is explained.

To analyze and optimize the dynamics of a new machine in the construction phase, finite element modelling is absolutely mandatory. For the purpose of optimizing a machine in an early stage of construction, quite rough models like the ones in figure 2 are sufficient. Fundamental machine behaviour results from the machine concept, which is defined by the masses to be moved, the kind of drives used and the collocation of all the masses, guideways and guide shoes. A finite element model of a milling machine (figure 2, left) is taken to explain some essentials of modelling machines whose axes are moved using ball screws or rack and pinion drives. To show the specifics of directly driven systems, a roll (figure 2, right) is taken as an example. It turns out that the integration of the encoder is essential for a good suppression of disturbances.

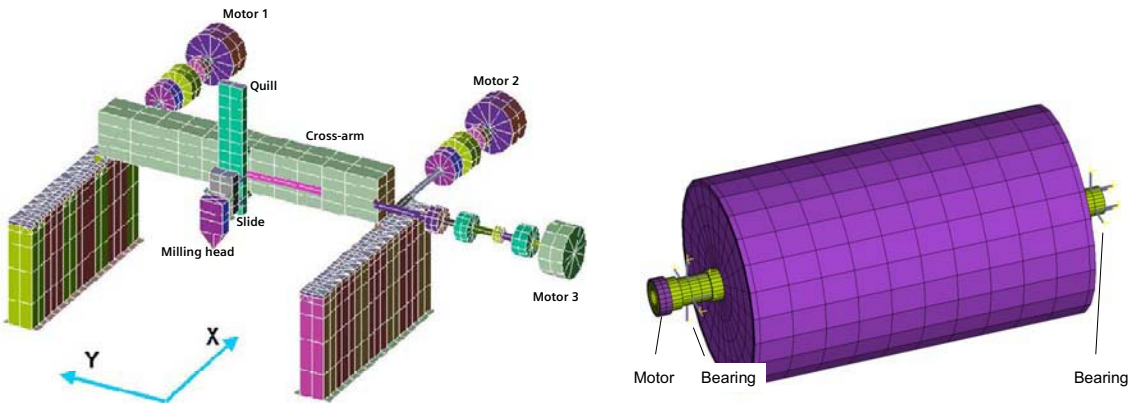

Figure 2: Finite element models of a milling machine (left) and a roll (right). Quite rough models are sufficient to detect weaknesses of a construction.

MODELING AND SIMULATION IN CONTINUOUS CASTING

Christian Furtmueller and Luigi del Re, JKU Linz, Austria
Karl Moerwald, VAI Siemens, Austria

Corresponding Author: Christian Furtmueller,
Johannes Kepler University,
Institute for Design and Control of Mechatronical Systems,
Altenberger Straße 69, 4040 Linz, Austria,
Phone: +43 732 2468 - 1873, Fax: +43 732 2468 - 9759
email: Christian.Furtmueller@jku.at

The average annual grows rate of steel production over the last 4 years has been 5.7% and in 2004 the world crude steel production has risen to an all-time high of 1057 million metric tons [5], particularly due to the enormous economic growth in China and other Asian countries. Especially continuous casting is used to solidify more then 90% of the steel produced in the world; and globally the fraction produced by continuous casting is still rising. Therefore enormous efforts in the design and control of continuous casting plants ([2] [3] [4]) have been made to increase throughput and quality of the product. Here mathematical modeling ([1] [6]) and simulation can be utilized to design and test controller before their implementation on the plant. The final aim is to increase quality and throughput and further provide safe commissioning.

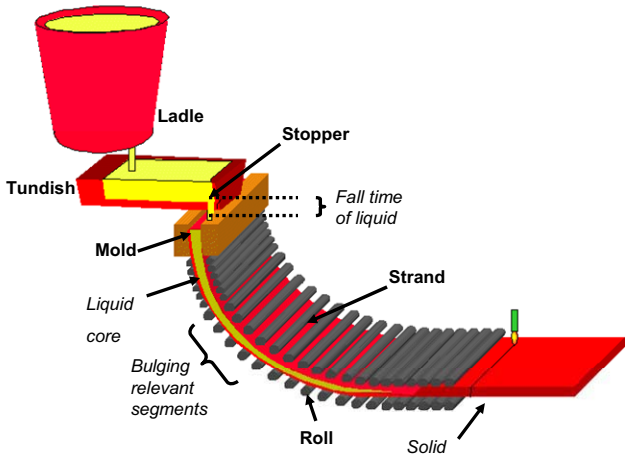

Fig. 1. Continuous casting plant

In this work we focus on modeling for controller design and simulation of the mold level regulation. Important uncertainty and disturbance effects are captured and new approaches [7] in this modeling are shown. In particular periodic disturbance effects as surface gravity waves and dynamic bulging are modeled and analyzed. The derived model can be used for controller design, controller validation and to test exceptional cases. It is also shown how the implemented software can be tested before the plant is put into operation and how the model can be used to improve the plant design.

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A SIMULATION PACKAGE FOR COORDINATED MOTION CONTROL OF A FLEET OF UNDER-ACTUATED SURFACE VESSELS

Filippo Arrichiello and Stefano Chiaverini, University of Cassino, Italy

Corresponding Author: F. Arrichiello
Università degli Studi di Cassino, DAEIMI,
Via G. Di Biasio 43, 03043, Cassino (FR), Italy
Phone: +39 0776-2994323, Fax: +39 0776-2993707
E-mail: f.arrichiello@unicas.it

The use of computer simulations is of self-evident importance when dealing with complex dynamical systems. Simulations allow to better understand the system's performance, to test and improve the control system design, and to avoid risky or costly operation in the preliminary stage of the system's design. Dealing with autonomous multi-vehicle systems, the use of a simulation tool allows testing different control strategies while achieving missions with different kinds of vehicles (e.g., ground vehicles, aerial vehicles, underwater vehicles, surface vessels, mobile robots, etc.) characterized by different kinematical and dynamical properties (e.g., fully-actuated or under-actuated, holonomic or nonholonomic vehicles).

To properly simulate an autonomous multi-vehicle system, both guidance system and vessel physic models have to be simultaneously taken into consideration. That is, the main dynamic parameters of the vessels (e.g., inertial generalized forces, hydrodynamic effects, environmental disturbances, actuation system) and control system characteristics (e.g., sampling time, saturations, thresholds, communication systems) should be considered.

In this paper a software package to simulate the motion of a fleet of autonomous surface vessels is presented. The proposed software, implemented in the MATLAB/SIMULINK environment, allows the user to test different supervisory control approaches, single-ship maneuvering control schemes, and dynamic models of the vessels in a number of missions for the fleet. At the present, the simulator has been widely tested with the guidance system proposed in [2], composed by a supervisor control derived from [1] and a maneuvering control derived from [4], while the vessels have a dynamic model derived from [3]. In particular, the considered vessels are fully-actuated at low velocities and under-actuated at high velocities; that is, the actuation system can perform forces in all the generalized directions at low velocities and in part of them at high velocities. Nevertheless, in the SIMULINK simulation scheme the user can easily change the parameters of the dynamic model, implement a different one, change the control schema (both the supervisor and the maneuvering control) or change the environmental conditions (inserting obstacles or adding forces representing wind, waves and current).

The simulator presents a graphical interface that allows the user to dynamically define all the parameters of the mission and the characteristics of the environment, e.g., the initial configuration of the fleet, the sub-tasks of the mission and their gains, the presence and the entity of environmental forces. For complex realistic mission, the presence of obstacles is also taken into account; thus, both punctual and continuous obstacles can be dynamically inserted in the environment to simulate costal profiles, reefs or other ships and rocks.

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ON FREE-FLYING REDUNDANT SPACE ROBOTS WITH NONHOLONOMIC CONSTRAINTS

B. Schäfer, B. Rebele and R. Krenn, DLR Oberpfaffenhofen, Germany

Corresponding Author: B. Schäfer
German Aerospace Center (DLR), Institute of Robotics and Mechatronics
Münchener Str. 20, D-82234 Wessling, Germany
Phone: +49 8153 28 1191, Fax: +49 8153 28 1450
email: bernd.schaefer@dlr.de

Free-floating manipulators in space exhibit nonholonomic behaviour due to their conservation of angular momentum. This implies that planning of robotic end effector trajectories and their control is highly complicated. In several studies this problem has already been investigated intensively, be it more from the kinematics and dynamics point of view or from control aspects. This complex trajectory planning task is more than ever valid if the manipulator degrees of freedom are increasing beyond the conventional number of six. Such kinematically redundant manipulators are favourably designed because of their flexibility in use and their increased skills. They are more and more intended to be applied in satellite servicing scenarios such as grasping of tumbling or malfunctioned target satellites in order to offer specific maintenance, berthing or even repair services. In these operational cases it is convenient for robotic task accomplishment, for instance in tele-operational and semi-autonomous robotic modes, to switch off the attitude and orbit control system of the chaser satellite where the robot is attached to. This free-floating satellite-robot compound system represents a very complex and flexibly moving system since the interaction between the robot motion itself and the satellite base is kinematically and dynamically highly coupled. Given a desired end effector (EE) trajectory of the manipulator in an inertial Cartesian frame, the accurate calculation of both the (actively) steered robotic joints and the satellite base passive variables is therefore a prerequisite for precise planning of satellite operational tasks with the robot in the loop.

In this paper we present two different approaches to solve for the compound motion behaviour that consists of $N+6$ degrees of freedom (dof), with $N>6$ for the redundant manipulator and 6 dof for the base. For both approaches the solution of the manipulator inverse kinematics (IK) is not as straightforward as in the conventional $N=6$ case with a robot fixed base. In the first approach (SBMM Superposition of Base and Manipulator Motions), solving for the overall motion dynamics, we subdivide the dynamics into two parts: first, a so-called relative part representing the influence of the manipulator relative to the satellite base (here, the IK problem of the redundant robot has to be solved for a fixed base first), and second, an absolute part representing the influence of the acceleration of the base due to the robot motion. In the second approach (IKCO Inverse Kinematics by Constraint Optimization), we regard the redundant manipulator with its satellite base, having the additional 6 dof as an entire, highly redundant robotic system for which we solve the IK problem by means of a Lagrangian based optimization technique. Here, we have to respect the desired EE trajectory given by its position and orientation sampled data along the prescribed trajectory, which is handled by corresponding constraints in the Lagrangian. Moreover, compared to a redundant robot attached to a fixed base, we now have to respect the two conservation laws of linear and angular momentum. This is achieved by regarding both laws as two additional constraints within the optimization algorithm. A typical simulation result is presented in Figure 1: It shows the calculated motion results of the two approaches for a 7 dof robot attached to a free-flying satellite base. In both approaches, the pre-scribed end effector trajectory is a circular path. The nonholonomic nature of the complete system is typically shown in the difference of the initial (lightly coloured) and the final configuration (boldly coloured) achieved after one closed loop.

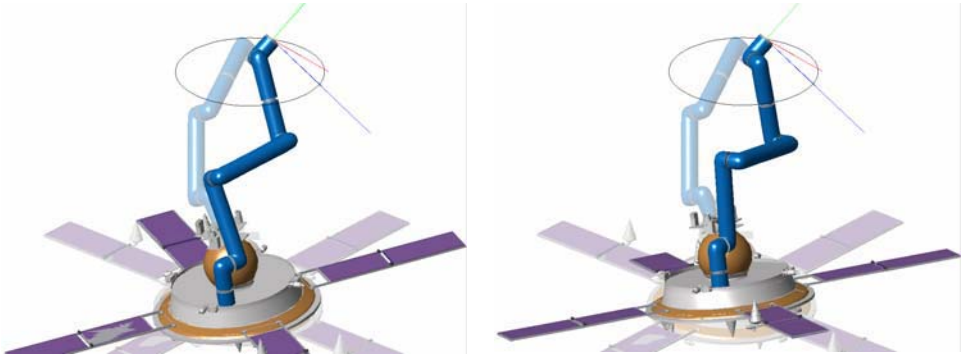

Fig. 1. Left: IKCO method (2nd order polynomial, sampling time $T_S = 1$ s); right: SBMM method (sampling time $T_S = 1$ s).

A MATHEMATICAL MODEL FOR THE PREDICTION OF THE MECHANICAL PROPERTIES OF AL-KILLED AND INTERSTITIAL FREE STEELS

V. Colla*, G. Bioli*, M. Vannucci*, R. Valentini°

*Scuola Superiore Sant'Anna, Pisa
°Materials and Metals Science Department of the University of Pisa
Corresponding Author: V. Colla,
Scuola Superiore Sant'Anna
Polo Sant'Anna Valdera, Viale R. Piaggio 34, 56025, Pontedera (PI), Italy
Phone: +39 050 883079, Fax: +39 050 883333
email: colla@sssup.it

This paper presents a mathematical model for the prediction of mechanical properties such as Ultimate Tensile Strength (UTS) and Yeld Strength (YS) for Aluminium-Killed and Interstitial Free steels.

Mechanical properties are quality parameters characterizing the fitness for use of rolled products. State of the art to determine yield strength and tensile strength is the selection of standardized specimens at the end of the process and destructive testing according to the definition in the inspection laboratory using standard tensile testing machines. Such kind of examination is obviously not satisfying for the producer because the material – per definition – is destroyed or locally damaged and because this kind of material investigation can be performed only statistically and not continuously online. Thus the development of a model capable o predicting properties such as UTS and YS is of utmost importance from the practical point of view and can provide the opportunity for considerable savings in terms both of time and of economical resources, as well as quality improvement, due to the possibility of continuous on-line monitoring. Therefore, the past decade has seen a number of workers in many countries developing mathematical models to predict the final mechanical properties of cold rolled and annealed metals [1, 2].

This paper presents a mathematical model based on the physics of the phenomenon under consideration, but also on the observations performed at the ILVA Works in Novi Ligure (Italy), where several data were collected. The model proposed in the paper has been designed to receive as inputs only data coming from the production line, and has been implemented through a software realised in the C++ programming language. An easy-to-use graphical interface allows to elaborate both the data referred to a single coil and a series of data referring to many coils stored into a database.

The experimental data collected on the plant have been exploited for tuning some of the model parameters by means of Genetic Algorithms [3]. The reason for adopting GAs instead of other optimisation techniques, such as the derivative-based ones, lies in the model complexity. The model requires the evaluation of a considerable number of equations that show a complex and highly nonlinear dependence on parameter values. Moreover, some conditional statements are present, i.e. the formulas that evaluate some of the quantities under consideration change depending on the ranges in which some input variables lie: the continuity is ensured but this is not true for the existence of the derivative. On the other hand, GAs require a huge number of model evaluations, thus the parameter optimisation through such technique can be very time consuming. A considerable effort was thus spent in order to optimise the code for the evaluation of the model so as to make it as efficient as possible and to avoid an excessive time consumption in the tuning phase.

The result of the optimization procedure, as well as the final model performance will be shown and discussed in the paper, by evaluating the results obtained in the processing of data coming directly from the industrial plants.

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Modelling for/and Control

ON STATE SPACE REALIZATION OF BILINEAR INPUT-OUTPUT DIFFERENTIAL EQUATIONS

Ü. Kotta[1], T. Mullari[1], A.S.I Zinober[2] and P. Kotta[1]

[1]Institute of Cybernetics at TUT
Akadeemia tee 21, 12618 Tallinn, Estonia
Phone: +372 6204153, Fax: +372 620 4151
emails: kotta@cc.ioc.ee, tanel@parsek.yf.ttu.ee, palle@cc.ioc.ee

[2] Department of Applied Mathematics, The University of Sheffield
Sheffield S10 2TN, UK
Tel: +44 (0)114 222 3888 Fax: +44 (0)114 222 3739
email: a.zinober@sheffield.ac.uk

The purpose of this paper is to find the subsets of continuous-time bilinear i/o equations

$$y^{(n)} = \sum_{i=1}^{n} a_i y^{(n-i)} + \sum_{i=1}^{n} b_i u^{(n-i)} + \sum_{i,j=1}^{m} c_{ij} y^{(n-i)} u^{(n-j)} \tag{1}$$

that are guaranteed to have a state space representation of order n, and as such are good candidate structures to be used in system identification, allowing in general, certain freedom in model structure selection. The results extend earlier results on realizability of discrete-time bilinear i/o equations [1]. Using a realizable i/o model is highly desirable for further control design since the state space description is central in modern nonlinear control theory.

Several equivalent necessary and sufficient realizability conditions in terms of advanced mathematical tools exist in the literature [2], that allow one to decide whether the bilinear i/o equation admits a state space representation or not. These conditions are not helpful if one wants to check realizability directly from knowledge of the bilinear i/o parameters a_i, b_i, c_{ij}.

The paper proves that the 2nd order bilinear i/o differential equation is always realizable in the classical state space form, unlike the discrete-time case. Necessary and sufficient conditions, in terms of restrictions on the bilinear model parameters, are provided to establish whether it is possible to find a state space representation of the i/o bilinear system or not for 3rd and 4th order models. When compared to the general realizability conditions, our conditions rely basically upon the property that certain combinations of coefficients of the i/o equations are zero or not. Since, even in low order cases, the necessary and sufficient conditions exhibit quite a peculiar and non-regular structure, it is a very difficult, and probably not a practical task, to find the necessary and sufficient conditions for the general higher order case. Instead, we suggest two subclasses of realizable i/o bilinear systems. Note also that earlier results do not suggest explicit state equations for realizable i/o models. Though a procedure to find them was given, the application, in general, requires integrating the integrable one-forms. This can sometimes be a complicated task. In this paper we provide explicit state equations for all realizable 2nd and 3rd order bilinear i/o equations, and for one realizable subclass of bilinear i/o equations of arbitrary order.

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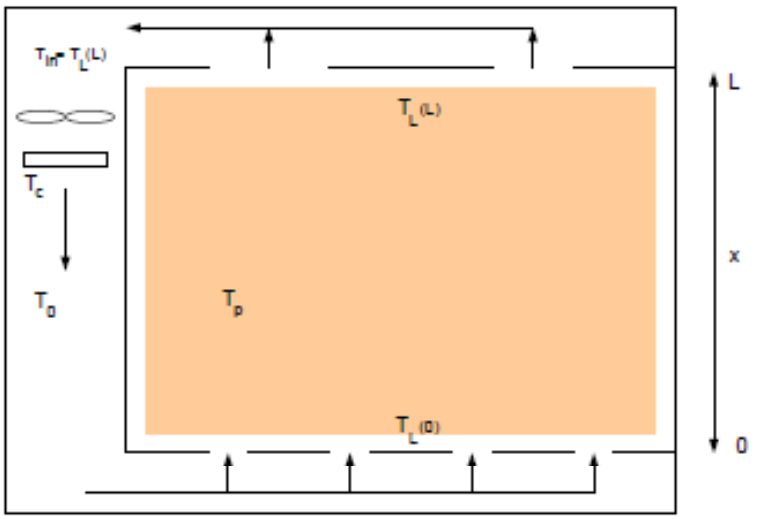
CLIMATE CONTROL OF A POTATO STORAGE ROOM

Corresponding author: S. van Mourik
Department of Applied Mathematics
University of Twente, The Netherlands
Phone: +31 (53) 489 3473 , Fax: +31 (53) 489 3800
e-mail: s.vanmourik@ewi.utwente.nl
S. van Mourik, H.J. Zwart

Abstract
A storage room contains a bulk of potatoes that produce heat due to respiration. A ventilator blows cooled air around to keep the potatoes cool and prevent spoilage. The aim is to design a control law such that the product temperature is kept at a constant, desired level. This physical system is modelled by a set of nonlinear coupled partial differential equations (pde's) with nonlinear input. Due to their complex form, standard control design will not be adequate. A novel modelling procedure is proposed. The input is considered to attain only discrete values. Analysis of the transfer functions of the system in the frequency domain leads to a simplification of the model into a set of static ordinary differential equations (ode's). The desired control law is now the optimal time to switch between the discrete input values on an intermediate time interval. The switching time can be written as a symbolic expression of all physical parameters of the system. Finally, a dynamic controller can be designed that regulates the air temperature on a large time interval, by means of adjustment of the switching time.



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A FAST ALGORITHM FOR TIME OPTIMAL CONTROL OF A COOPERATIVE MULTI MANIPULATOR SYSTEM ON SPECIFIED PATH

Mohammad J. Sadigh and Mohammad H. Ghasemi

Corresponding Author: Mohammad J. Sadigh
Mechanical Engineering Department, Isfahan University of Technology,Isfahan, Iran
Phone: (9821) (33114907) Fax: (9821) (33114247)
Email: mjsadigh@istt.org

A Cooperative multi manipulator system (CMMS) is defined as a system of multiple robots handling a common object (Figure 1). Time optimal motion of CMMS is an interesting subject which has been studied by several researchers. Bobrow et al.[1] proposed a method for time-optimal control of robotic manipulators along specified path. McCarthy and Bobrow, [2], proved that for a manipulator with *n* coordinate, *p* differential constraint equations and *m* actuators, at least *m-n+p+1* actuators are saturated during a time optimal motion along a prescribed path. Moon and Ahmad [3], employed a similar algorithm to find the time-optimal trajectory for a cooperative robot. They showed that to find the maximum and minimum values of acceleration at each point, one should solve a linear programming problem, which makes the solution very costly.

In this paper we proposed a method to reduce calculation effort for minimum time control of a CMMS along specified path. The method takes advantage of the number of saturated actuators at each step and reduces the linear programming problem needed for calculation of extremum into the solution of a linear set of equations. More detailed studies are carried out about the characteristics of locked area of phase plane, to which no solution can enter, and trapped area, from which no solution can escape, see Figure 2. This study shows that the lower boundary of locked and trapped area is the switching curve construction of the switching curve cuts the calculation efforts further. Reducing the computational effort, the method presented in this paper can help to develop an online control algorithm for minimum time movement of a CMMS along a prescribed path which, of course, need further studies

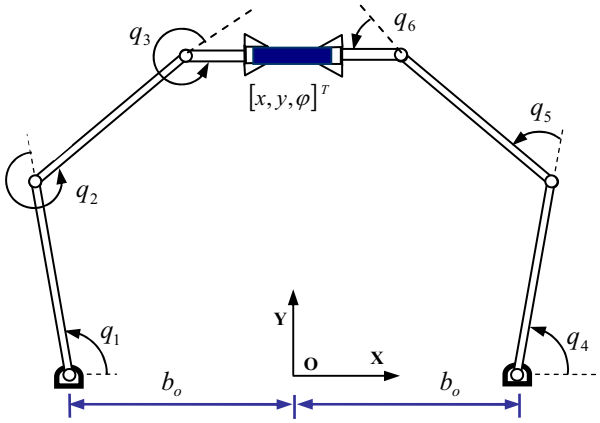

Fig 1. schematic diagram of the CMMS

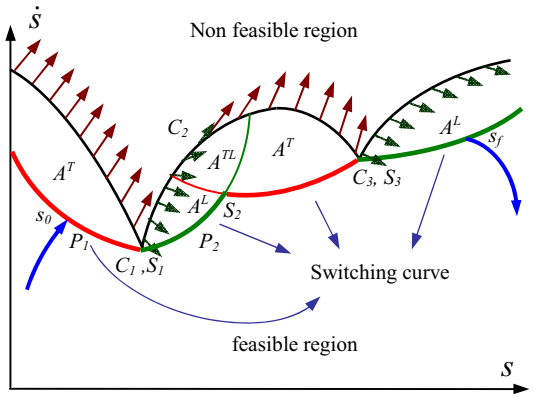

Fig 2. schematic diagram of switching curve

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MODELING, VALIDATION AND OPTIMAL CONTROL OF CONSTRAINED NONLINEAR OIL TANKER MOTION

Tayfun Çimen* , TNRCC – Istanbul, Turkey

Turkish Naval Research Center Command
Ankara Caddesi, No: 252, 34890 Pendik – Istanbul, Turkey
Phone: +90 538 3161356, Fax: +90 216 4938287
email: tcimen@roketsan.com.tr

Maneuverability is of great importance for large tankers in the marine industry. Oil transport through narrow channels involves serious risks, which need to be carefully assessed and analyzed. Maintaining position within the lanes becomes difficult for large tankers, if not impossible. The Strait of Istanbul (Bosporus), for example, is unique in many respects. The very narrow and winding shape of the strait route makes ships traveling through the Bosporus more akin to that of a river, necessitating at least twelve course changes to avoid running aground. There have been hundreds of accidents over the past decade, resulting in loss of life and series damage to the environment. The major causes of accidents were insufficient maneuvering or stopping room due to traffic congestion, and adverse environmental conditions such as fog and cross currents. Navigation safety in such channels, therefore, requires precise knowledge of maneuvering behavior of the ship under the effects of water depth, channel bank, and environmental conditions such as wind, wave and/or current. In particular, supertankers are manually difficult to handle due to their massive size, since large variations in the steering characteristics can appear suddenly. Therefore, autopilots that can be used to make accurate course changes in narrow coastal waters, such as the Bosporus, are of great importance.

A great deal of effort has been devoted to the construction of nonlinear mathematical models describing the maneuverability of large tankers in deep and confined waters in the general state-space form $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u})$. The maneuverability performance of one of these models, the ESSO 190,000-dwt tanker, involving the ship control system has been investigated in [3] using full-scale trial results. In this paper, nonlinear and coupled motions of the heading and propulsion dynamics of large tankers are derived and validated using results from full-scale sea trials of [3]. The effect of the rudder on the turning dynamics of the ship is then investigated. Unfortunately, the classical model used for representing the flow velocity at the rudder is seen to respond much more rapidly than is physically possible for an oil tanker of the size considered in [3], thus obscuring one of the most significant characteristics of large tankers, that is, the length of time taken to respond to forces acting upon the ship. There is strong evidence that the standard model, which has been used in the literature on ship dynamics for more than three decades, is *not* representative of the motions of a real tanker. As a consequence any control system designed using this "fast" model benefits from the improved speed of reaction and increased turning moment produced by the rudder. However, the controller performance derived from simulation results will be greatly reduced when applied to a real tanker. In order to compensate for this increase, a new rudder model was recently proposed in [2], which is superior over the classical model and describes the physical system much better. It is, therefore, imperative to alert readers interested in marine applications to the existence of this type of modeling errors, since similar errors are also present in other papers in the literature [4].

Using a recently proposed method for nonlinear optimal tracking control [1], a course changing controller based on the proposed model is designed for the unconstrained problem. Results are presented taking into account actuator saturation in the rudder angle and rudder rate. The proposed feedback algorithm is modified in order to constructively impose hard constraints of rudder rate saturation into the design process.

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* Currently with ROKETSAN Missiles Industries Inc., Engineering Development Group, Elmadağ – Ankara, Turkey.

MODELING AND CONTROL OF AN ELASTIC SHIP-MOUNTED CRANE USING VARIABLE GAIN MODEL-BASED CONTROLLER

Yousef Al-Sweiti and Dirk Söffker

Corresponding Author: Yousef Al-Sweiti
University Duisburg-Essen, Engineering Faculty
Chair of Dynamics and Control
Lotharstraße 1, 47057 Duisburg, Germany
Email: alsweiti@uni-duisburg.de

Abstract
This paper deals with mathematical modeling and control of elastic ship-mounted cranes equipped with the Maryland Rigging. The model contains three independent inputs to control the vibrations in the plane of the boom due to the rolling disturbance of the ship; the luff angle is proposed to control the elastic vibration in the boom, and the total length of the upper cable in conjunction with the position of its lower suspension point are proposed to control the pendulation of the payload. The disturbance acting on the ship due to sea motions is represented by the rolling displacement of the ship about its center of gravity. The full nonlinear model of the crane is developed and Taylor series is utilized to expand the nonlinear terms about the current equilibrium point which vary with the luff angle and the length of the upper cable. This leads to a linear model with all nonlinear terms (higher order terms) collected in a separate column vector. Simulation results show that, within a considerable range of pendulation displacements of the payload the nonlinear model and the linearized one obtained by dropping the nonlinear terms from consideration reflect nearly equivalent responses. Consequently, the linear model is used to design the control system of the crane. The coefficient matrices of this linear model are calculated at the current (instantaneous) equilibrium point, which vary with the luff angle and the length of the upper cable, therefore, a variable model problem is created and accordingly a variable gain observer and a variable gain controller are designed to cover the operation of the crane for all possible equilibrium points in the working space. The switching action between these gains takes place automatically according to the output of a region finder, which uses the measurements of the luff angle and the length of the cable to detect the current operating region. PI-Observer is used to estimate the states and the unknown disturbance force acting directly on the payload; this improves robustness of the observer and guarantees that the estimated states converge to their real values even though a nonzero disturbance force acts on the payload. The controller uses the estimated states and the measured roll angle to create the required active damping and to compensate for the rolling action of the ship. Stability and performance robustness of the system are ensured for the total working space and also for the expected range of the payload mass. Simulation results show that the observer can estimate the states and the unknown disturbance acting on the payload very well and the controller can reduce the payload pendulations significantly.

Underground Analysis, Prognosis and Control, based on modern ICT Methods

Dietmar P. F. Möller*, Christian Körber, Christian Zemke,
University of Hamburg, Department Computer Science, Chair Computer Engineering (AB TIS),
Vogt Kölln Str. 30, D-22527 Hamburg, Germany
email: dietmar.moeller@informatik.uni-hamburg.de
Caroline Hanusch, Klaus Maas,
Technical University of Clausthal, Germany

Underground analysis in general is based on the geo-scientific approach, that often belong on geo-technical and/or geo-mechanical component representations. Such representations are 2D or 3 D geo-models or geo-objects, containing normally area or spatial data and in some cases temporal data. Due to the requirements of the geo-scientific problem under test, which is in the on hand abstract the underground analysis, prognosis and prediction, a specific geometrical modelling approach has to be chosen. In general it can be stated that one model for instance might support differential geometry very well, but it may lack the ability to interpolate complex geometry, while another model may fit better, while lacking in differentiability, etc.
For this reason this paper will focus on common geometrical models in the context of modelling the important process of salt leaching in flooded potassium mines. Emphasis is taken due to model topology and model dynamics. These dynamic interactions can be localized along the so called reaction surface between brine (fluid) and rock (solid), more basically between objects with different geochemical attributes. The direction and velocity of the solution process can be described by vectors, determined by an underlying process model, that integrates the relevant parameters of all involved objects (rock, fluid, reaction surface). Hence, the basic requirements for a geometrical model (the term model refers to 2- and 3D geometrical models) being capable to represent the described features as follows:

- Many complex bodies
- Dynamically altering objects
- Differential geometry on the reaction surface
- Interactions/interdependencies between objects
- Topology preservation (no self penetration etc.).

Due to the several degrees of freedom (control points, knot vectors, weights) the chosen parametric model provide, complicate controlled model modification, which is especially significant for NURBS (Non Uniform Rational B-Splines). This special kind of B-Spline representation is based on a grid of defining points $P_{i,j}$, which can be approximated through bi-cubic parameterized analytical functions. Based on this approach is it possible to calculate the resulting surface or curve points by varying two (surface) or one (curve) parameter values u and v of the interval [0,1], respectively, and evaluating the corresponding B-Spline basis function $N_{i,p}$. Hence, a geometrical model that support the several properties has been invented.
Assuming that we have determined the leaching cells, we can compute the mass-volume exchange between fluids and solids by chemical-thermodynamic equilibrium balances. But still no kinetic or mechanic influences are involved in the leaching approach. Hence we combine the geochemical computer model with a specific rule based system, that is embedded in a specific GIS architecture.

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MODELLING QUADRATIC SUBOPTIMAL CONTROLLERS FOR DYNAMIC INTERCONNECTED BILINEAR SYSTEMS

M. de la Sen[†], Aitor J. Garrido[‡], J.C. Soto[‡], Oscar Barambones[‡], Francisco J. Maseda[‡], Izaskun Garrido[‡] and Asier Ibeas[*]
Corresponding Author: Aitor J. Garrido
[†]Institute of Research and Development of Processes (IIDP). Dept. of Electricity and Electronics. Faculty of Science and Technology. University of the Basque Country. Leioa (Bizkaia), Apdo. 644 de Bilbao. 48080 SPAIN
http://www.ehu.es/IIDP/delasen
[‡] Dept. of Systems Engineering and Automatic Control. EUITI de Bilbao. University of the Basque Country. Bilbao (Bizkaia), Plaza de La Casilla. 48012 SPAIN
[*] Dept. of Telecommunications and Systems Engineering. Escuela Técnica Superior de Ingeniería. Universidad Autónoma de Barcelona. Campus de Bellaterra, Edificio Q. 08193 SPAIN
email: {manuel.delasen, aitor.garrido, juancarlos.soto, oscar.barambones, fcjavier.maseda, izaskun.garrido}@ehu.es; Asier.Ibeas@uab.es

Abstract. This paper focuses on the suboptimal regulation of multivariable discrete-time bilinear systems consisting of interconnected bilinear subsystems with respect to a linear quadratic optimal regulation criterion which involves the use of state weighting terms only. Three transformations are used in order to treat the scheme over an equivalent linear model. This leads to the appearance of quadratic weighting terms related to both transformed input and state variables. In this way, a Ricatti matrix-sequence allowing the synthesis of a standard feedback control law is obtained.

1. Introduction

This paper reports the modelling of quadratic suboptimal controllers, which are applied to bilinear models using optimization techniques. First, the system is shown to be equivalently described by the linear feed-forward multivariable structure with multiplicative inputs including a deterministic disturbance vector. As a previous requirement for optimization, controllability results for the overall systems performance are given. This is achieved through the use of centralized control methods. In this sense, two suboptimal control models are developed and applied to certain classes of invariant discrete-time multivariable bilinear systems with interconnection subsystems. An unusual explicit solution of Ricatti type is found out as the suboptimal solution by using manipulations on the input/state variables of the problem statement. The importance of this strategy arises from problems where constrains on the input rather than input weights are introduced in the optimization criterion, what leads to a feedback-type control law. Therefore, the proposed technique allows to deal with multiple problems which are bilinear and involve interconnections.

2. Models for a class of bilinear systems with interconnected subsystems

In this paper, the following typical class of bilinear systems is considered:

$$x(k+1) = \left[A + u(k)B\right]x(k) + Cu(k); \qquad k = 0,1,2,\ldots,\ x(.) \in R^n;\ u(.) \in R \tag{1}$$

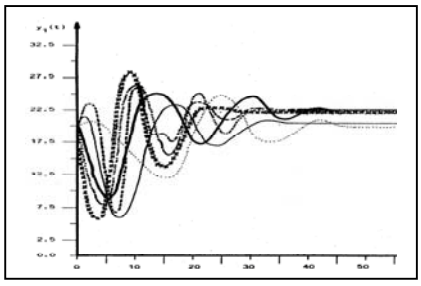
where $x(k)$ and $u(k)$ are the state and the control at time k, respectively; and, A and B are real constant coefficient matrices of compatible dimensions, from which an equivalent multivariable structure discrete model is obtained.

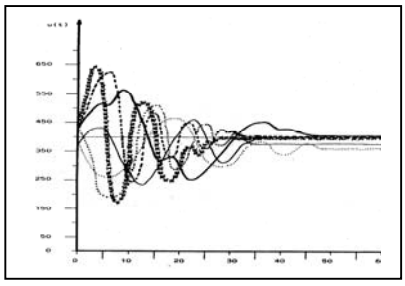
3. Suboptimal control models

Then, a regulation model which involves quadratic weighting terms in the state variables is given. The philosophy involved is to define transformed state and input variables. Its major interest appears in the case of constrained input sequences because, a recursive Ricatti expression can be found leading to the optimal feedback solution.

4. Numerical Simulation

It may be observed that the approaches applied have effect only on the system implementability rather than on its stability while providing the desired control results.





5. Conclusions

A multivariable invariant discrete-time bilinear system being composed of interconnected subsystems has been studied obtaining an equivalent feed-forward linear model with equivalent inputs, which are derived from products state-input. Then, the system has been controlled with respect to a quadratic finite-time optimization horizon in order to drive each subsystem from any arbitrary initial point to a predefined final state using different suboptimal control models. It is shown that the suboptimal controllers modelled provide appropriate control results.

Acknowledgment

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BUILDING AN UNKNOWN INPUT OBSERVER (UIO) FROM A BOND GRAPH MODEL: A GEOMETRIC APPROACH

César Pichardo-Almarza[2,3], Ahmed Rahmani[1], Geneviève Dauphin-Tanguy[1]

Corresponding Author: César Pichardo-Almarza
[1] Ecole Centrale de Lille, L.A.G.I.S. UMR CNRS 8146, BP 48. 59651. Villeneuve d'Ascq Cedex, FRANCE.
Phone: +33 (0) 3 20 33 54 15, (Fax: 54 18)
[2] University of Sheffield, Computer Science Department, 211 Portobello Street, Sheffield S1 4DP, U.K.
[3] Universidad Simon Bolivar, Caracas 89000, VENEZUELA
e-mail: pichardo.cesar@ec-lille.fr

In this paper some geometric tools were used to build an unknown input observer (UIO). This is a first contribution to design observers using a geometric approach and bond graphs. Some previous works propose graphical techniques (based on algebraic approaches) to design observers from a bond graph model [3 – 4].
The geometric approach defines tools for the structural analysis and control of linear systems. In fact, it consists on associate the dynamical properties of the system to the space properties.
Our main objective is to develop an approach to calculate an observer which decouples the unknown perturbations from the state estimation. We have used some results proposed by [2]. These authors used a geometric approach to calculate a decoupling control law from a bond graph model.
We consider a Luenberger observer when the system has known inputs (u) and unknown inputs (d):

$$\begin{aligned} \dot{x}(t) &= Ax(t) + Bu(t) + Ed(t) \\ y(t) &= Cx(t) \end{aligned} \quad \Rightarrow \quad \begin{aligned} \dot{\hat{x}}(t) &= A\hat{x}(t) + Bu(t) + G(\hat{y}(t) - y(t)) \\ \hat{y}(t) &= C\hat{x}(t) \end{aligned} \tag{1}$$

Model of the system *Luenberger Observer*

The differential equation of the estimation error, $e = \hat{x} - x$, is :

$$\dot{e}(t) = (A + GC)e(t) - Ed(t) \tag{2}$$

Equation (2) shows that the estimation error does not converge asymptotically to zero, even if the matrix (A + GC) is stable. However, this error converge asymptotically to the subspace $S^* = \min S(A+GC, \mathrm{Im}(E))$, i.e., to the reachable set of system (2). Thus, to obtain the best state estimation, we must select G such that this subspace has the minimal dimensions. Because of S^* is a ($\boldsymbol{C}$,A)-invariant subspace, the best selection of G corresponds to transform the ($\boldsymbol{C}$,A)-invariant subspace containing Im(E) in a (A+GC)-invariant subspace (structural condition linked to the possibility to estimate the states if the initial conditions of the system and the observer are congruent [1]) or the minimal ($\boldsymbol{C}$,A)-invariant subspace externally stabilisable containing Im(E) (condition of stability that guarantees the convergence of the estimated states to the actual states, even if the initial states are not congruent). In the last case, the interne stabilizability of the conditioned invariant is implied by the supposition that (A,C) is detectable, which is clearly necessary if we consider a full order Luenberger observer. This state estimation may be satisfactory if, for example, we do not need to know all the state vector, but only a linear function of the states: in this case, the asymptotic estimation of this function is possible if only if S is contained in its kernel [1].
The methods to design a Luenberger observer able to reject a non-measurable perturbation are based on the classical concepts of invariant subspaces, in particular ($\boldsymbol{C}$,A)-invariant subspaces are used. This approach allows calculating the observer gain using causal manipulations from the bond graph model of a system without necessity of writing the state equations. The paper is organized as follows: Section 1 gives some basic concepts of the geometric approach needed for the design of the observers. Section 2 presents two methods for building the unknown input observers from a bond graph model. Section 3 shows an example where we apply the methods for building an observer. Finally Section 4 gives the conclusions of this work.

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INTERMITTENT AND PERIODIC OBSERVATIONS IN KALMAN FILTERING

Luciano Carotenuto and Paolo Pugliese

D. E. I. S., Università della Calabria
via P. Bucci, 42/C, 87030 Rende, Italy
(carotenuto@unical.it, pugliese@unical.it)

In a recent paper [1] the state estimation of a linear stochastic system for which observations occur randomly has been considered. This reflects the practical situation where measurements may be lost because of connection failures between the sensors and the controller. This scenario is becoming more and more relevant because of many applications where a network of sensors is connected to a controller through wireless links. The system we consider is discrete time, n-dimensional, p-output:

$$\begin{aligned} x_{k+1} &= A\,x_k + w_k \\ y_k &= Cx_k + v_k, \end{aligned}$$

the input w_k being a zero-mean, white Gaussian noise with covariance matrix $W > 0$.

The measurement noise v_k models the acquisition or the loss of a new observation: v_k is a white, zero-mean Gaussian sequence whose variance is defined according to the values a Bernoulli random variable γ_k takes:

$$\begin{aligned} E[v_k v_k' \mid \gamma_k = 1] &= V, \qquad Pr\{\gamma_k = 1\} = \lambda \\ E[v_k v_k' \mid \gamma_k = 0] &= \sigma^2 I, \qquad Pr\{\gamma_k = 0\} = 1 - \lambda, \end{aligned}$$

with $V > 0$, σ^2 a large positive number, and γ_k independent of γ_s for $k \neq s$. The rationale of the model is that the lack of observation is equivalent to an observation corrupted by a large (infinite, in the limit) noise.

A Kalman filter can easily be built up to cope with this context: see [1] for the details. The fundamental difference from the standard Kalman filter is that the filter gain and the prediction error covariance matrix are now random matrices. Moreover, a critical value λ_c there exists such that if $\lambda < \lambda_c$ and the system is unstable then the mean of the prediction error covariance matrix is unbounded.

We compare the state estimation problem when measurements *may arrive* with probability λ with the case of measurements that *arrive* any $N = 1/\lambda$ instants, assumed integer. To this purpose, consider the output transformation

$$\Gamma_k = \begin{cases} C & \text{for } k = 0, N, 2N, 3N, \dots \\ 0 & \text{otherwise.} \end{cases}$$

This is a special case of a periodic system: for such systems it has been proved in [2] that if the time varying pair (A, Γ_k) is observable then the state estimate converges to a ciclostationary random sequence, whose covariance matrix is symmetric periodic of period N, hence bounded.

There is then a deep difference between the case of regular observations with period $N = 1/\lambda$ and the case of random observations with probability $\lambda = 1/N$. The aim of our work is to investigate this difference further.

In particular, we re-derive some results of [1], and obtain some new ones, using a probabilistic approach, that gives more insights on the behavior of the process $P_k = E\{(\hat{x}_{k|k-1} - x_k)(\hat{x}_{k|k-1} - x_k)'\}$, where $\hat{x}_{k|k-1}$ is the prediction of the state at the time k based on the observations $\{y_1, \dots, y_{k-1}\}$, some of which may be pure noise.

Let k_0 and $k_0 + d$ be two successive instants at which observations occur, $d \geq 1$, and let S_{k_0} be the covariance matrix of the state estimate $\hat{x}_{k|k}$, obtained after the output y_k has been processed:

- For first order systems we compute the expected value and the distribution of P_{k_0+d} conditioned on S_{k_0}.
- For systems of order $n > 1$ we give some results about the boundedness of $E\{\text{tr}(P_{k_0+d}) \mid S_{k_0}\}$.
- If the output matrix C is square and nonsingular, we show that the a-posteriori covariance S is bounded independently of the sequence of observations.

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Nonlinear Oscillations

Torus Breakdown and Chaos in a System of Coupled Oscillators

Taoufik Bakri

Abstract

In this paper, we consider a simple system of two nonlinearly coupled oscillators using averaging and numerical bifurcation techniques. Assuming the internal resonance 1:2 and the coupling terms having opposite sign we establish the existence of a 2π-periodic solution which undergoes a supercritical Neimark-Sacker bifurcation, yielding a stable fixed symmetric torus. Through one route in the parameter space, we numerically show how the torus gets destroyed by numerically following the changes in the involved manifolds. We detected a cascade of period doubling within the 1:6 resonance tongue yielding a strange attractor. Other periodic regimes present in this system are also studied. It seems these two different regimes interact with each other, yielding yet another type of strange attractor. All this happens quite far from the origin. Most of the results in this region are numerical. Still interesting phenomena were captured by the numerical packages CONTENT, AUTO and MATCONT showing the complex character of the dynamics in this simple system of coupled oscillators.

STRANGE BEATING BEHAVIOUR OF A DRY-FRICTION OSCILLATOR

Gábor Csernák, HAS-BUTE Research Group on Dynamics of Machines and Vehicles
Gábor Stépan, Budapest University of Technology and Economics

Corresponding Author: G. Csernák,
Budapest University of Technology and Economics,
H-1521 Budapest, Hungary
Phone: +36 1 463 1332, Fax: +36 1 463 3471
E-mail: csernak@mm.bme.hu

A harmonically excited dry friction oscillator is examined analytically and numerically in this paper. We search for $2\pi/\Omega$-periodic non-sticking solutions, where Ω is the excitation frequency. Using the assumption that there are only two turnarounds during each cycle, we prove that the motion is symmetric in space and time at almost all the values of Ω, but there are special parameters, where an infinity of marginally stable, asymmetric solutions coexist. We point out that a strange beating phenomenon may cause quite large numerical errors close to resonance.

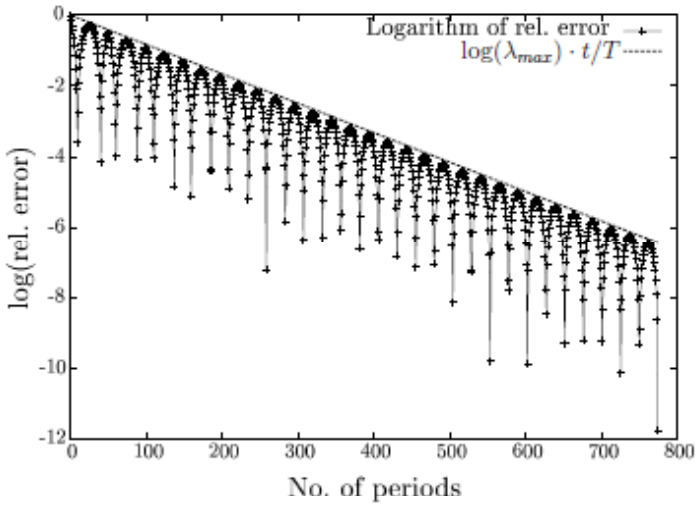

Figure 1: Convergence to the symmetric solution at $S = 0.1$ and $\Omega = 0.98$

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Hydraulic Switching Control with Nonlinear Converters

R. Scheidl, B. Manhartsgruber, JKU Linz, and H. Kogler LCM, Linz, Austria

Corresponding author: R. Scheidl
Johannes Kepler University, Linz, Austria
Altenbergerstrasse 69, 4040 Linz, Austria
Phone: +43 732 2468-9745 Fax: + 43 732 2468-9753
email: rudolf.scheidl@jku.at

Hydraulic switching control attempts to transfer analogous concepts from modern electrical drive control to hydraulics. A one to one copy of electrical concepts is inhibited by some specific properties of hydraulic systems, in particular the displacement principle of hydrostatic machines which is dual to electrical machines, the inability to realise a pure hydraulic inductivity, the cavitation phenomenon, the missing of extremely fast valves, and the nonlinear characteristics of hydraulic accumulators. These facts require a more thorough analysis of hydraulic switching converters.

In this paper, the hydraulic analogy of the so called `Buck Converter` of power electronics is studied. This converter consists of a discrete inductivity and capacity and a valve. In our system, the capacity is realised by a standard gas spring hydraulic accumulator with a nonlinear behaviour and the inductivity by a hydraulic pipe. Switching is done by two 2/2 way valves, one for the high and low pressure supply port. For suppression of cavitation, an additional small accumulator is inserted between the two valves and the pipe. The electrical `Buck Converter` represents one of the simplest converter types, its behaviour is easy to understand. Its hydraulic pendant, however, is much more complex in nature, due to the differences mentioned above.

The task to be solved here is to work out the simplest model (a reduced model) for this converter configuration, which describes the essence of its behaviour, and, additionally to find the ranges in parameter space of the complex system for which this reduced model is valid. First, a simplified model comprising the small accumulator as a nonlinear spring, the larger accumulator as a pressure boundary node, a pure hydraulic inductivity, reflecting the inertia properties of the pipeline, and the valves with ideal switching performance is studied. This is considered a reduced model of the real system if compressibility of the hydraulic fluid is neglected and the accumulator's hydraulic capacity is considered infinite.

The behaviour can be geometrically studied in a phase plane with the co-ordinates pressure in the small accumulator and the flow rate in the pipe overlaying the trajectories of the two switching states high or low pressure port on. Both switching states have one globally attracting singular point. For small accumulator capacities, they furthermore exhibit a one dimensional invariant manifold which characterises a slow dynamics of the system, characterised by a nearly constant pressure and increasing (high pressure on) and decreasing (low pressure on) flow rate. The practical relevant remaining part of the phase space is "foliated" by trajectories representing the fast dynamics of the reduced system. Hydraulically, this is a nearly constant flow rate but a changing pressure. Approximate simple formulas are given to describe both type of trajectories and the flow on them. With these results, the reduced system can be evaluated w.r.t. the technical requirements.

In a second step the question is investigated, under which circumstances the disturbed system, i.e. the system taking into account the complex dynamics of wave propagation in the pipe, the finite capacity of the large accumulator, the finite switching time of the valves, and the dynamical properties of an attached hydraulic cylinder, is close to the reduced system. From a system design point of view this means that these effects do not violate those characteristics of the system behaviour which are essential for its technical performance. This investigation is done numerically. The pipeline dynamics is modelled by a method characteristics accounting of the frequency dependent friction behaviour of the fluid. Results are visualised in a specific modified phase space, being the product space of the phase plane of the reduced model and appropriate norms indicating the deviation of the complex from the reduced model.

Numerical Continuation of Fixed Points of Maps in CL_Matcont

Hil G.E. Meijer
Mathematisch Instituut
Universität Utrecht
Budapestlaan 6, PO-Box 80010
3508 TA Utrecht, Netherlands

tel:+31-(0)302531527
email:hmeijer@math.uu.nl
www.math.uu.nl/people/hmeijer/

Abstract :
We discuss a new continuation environment for discrete-time dynamicalsystems: `CL_Matcont'. It is a Matlab Toolbox and is based on Content[1], but many parts are rewritten. Apart from evaluating orbits, it facilitates continuation of codimension one
bifurcation curves with respect to two paramters. Along such curves extra degeneracies,
codimension 2 bifurcations, occur in generic 2-parameter families. Two new aspects of the toolbox are the automated normal form analysis of such codim-2 bifurcations and branch switching to local codimension one bifurcations rooted at codimension 2 points. These aspects are discussed in more detail.

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Modelling in Biology and Physiology

Modelling nectar-collecting behaviour in a honeybee colony

R. Thenius, T. Schmickl and K. Crailsheim
University of Graz, Austria

Corresponding Author: R. Thenius
Department for Zoology
Universitätsplatz, 8010 Graz, Austria
Phone: +43 316 380-8759; Fax: +43 316 380-9875
email: theniusr@stud.uni-graz.at

Honeybees have to collect nectar in the environment to accommodate their energetic demands. The collection of nectar is performed by a special cohort of bees: the forager bees. These bees fly in the environment and collect nectar from flowering plants. Returning forager bees transfer the collected nectar to another special cohort of bees (storer bees) inside of the colony. These storer bees then store the nectar in honeycombs inside the colony. A returning forager bee does not always transfer its whole nectar load to one single storer bee but to several storers. This process is called "multiple unloading". The probability of the occurrence of such multiple unloadings correlates with the mean crop load of the returning forager, due to a mismatch between the crop load of the foragers and the available empty space in the crop of the storer bees.

The mean crop load of the returning foragers is influenced by environmental conditions during the foraging trip. Under conditions of low natural nectar flow in the environment (only little amounts of nectar available) forager bees return with small amounts of nectar from their foraging trips. Under conditions of high natural nectar flow, that is big amounts of nectar available in the environment, forager bees return with almost full nectar crops to the colony. A honeybee colony can differentiate between several nectar sources in the environment, and it exploits massively the most profitable source. Our goal was to find out, if bees that are foraging on one source may detect changes in the nectar flow of another source without visiting this source by themselves.

Our simulation focuses on several aspects of honeybee foraging: on the dynamics of the crop load volume during a foraging trip, on the distribution of crop load volumes under different environmental conditions, and on changes in the frequency of multiple unloads, caused by changes in the environmental conditions. Our simulated honeybees are represented by agents implemented as finite state automatons. Each simulated honeybee has its own metabolism, using nectar as energy source. Biometric data of the honeybees like weight, metabolic rate, crop volume, and flight speed were taken from literature.

Our studies show that a group of foraging bees is able to detect changes in the natural nectar flow on alternative sources which they are not currently exploiting by themselves. This communication works indirectly via the cohort of storer bees, using two channels of communication: on one hand, there is a small change in the amount of multiple unloads experienced by the forager bees, on the other hand, there is an increase of the searching time of the returning forager bees for storer bees. We show that foraging bees have more information available about the current status of the environment as previously thought.

The transfer of information between single bees as well as between groups of bees is very important in a decentralised system like a honeybee colony. Honeybees have to optimise their foraging decisions without any central processing unit. Therefore the amount and the quality of information available to each single forager bee is of big importance in this decision making process. For a general understanding of this decentralised natural system it is of crucial to know all channels of communication within the system. These findings of yet unknown additional channels of information call for further investigation, using empirical experiments as well as simulation techniques. With the work at hand we show that our simulation is a valid tool to investigate internal mechanisms that regulate foraging of honeybee colonies and to study the pathways of information in such a decentralised insect society.

MODELLING THE SELF-ORGANIZED DIVISION OF LABOUR IN HONEYBEES

T. Schmickl and K. Crailsheim, Karl-Franzens-University Graz, Austria

Corresponding Author: T. Schmickl
Karl-Franzens-University Graz
Universitätsplatz 2, 8010 Graz, Austria
Phone: + 43 316 380-8759, Fax: + 43 316 380- 9875
email: schmickl@nextra.at

In eusocial insect colonies (ants, termites, wasps, honeybees) up to tens of thousands of workers live together as a precisely regulated superorganism. Such a superorganism is able to respond to environmental fluctuations, it is able to achieve internal homeostasis and it shows intelligent collective behaviour ("swarm intelligence"). These collective abilities are achieved by the assessment of local information perceived by individual workers, which show specific task-related behaviours in response to these stimuli. In social insect colonies, the phenomenon of division of labour is observed frequently. This division of labour is mainly achieved via specialisation of workers for specific tasks, but this preferential allocation of workers to task cohorts is usually flexible.

We present here a multi-agent model of a honeybee colony. In this multi-agent model, each individual bee is represented by an own process (agent), which determines the behaviour of the agent. Theses agents respond (like all living things do) to stimuli in their local surrounding. Their behaviour can change their local environment, thus changing the stimuli perceived by other agents: This way a network communication arises within the system, allowing self-organisation to happen. Our model **TaskSelSim** focuses on the flow of nectar within a honeybee colony. Nectar is a resource that is collected by a special task cohort of bees in the outside environment. These forager bees return to the nest and handle the nectar over to another cohort of worker bees, called nectar storage bees. These storage bees transport the nectar to the honey comb and store it into cells. Nursing bees collect the nectar from these cells, digest it and feed the derived carbohydrates to the brood. All bees (foragers, storers, nurses and brood) metabolize the nectar to satisfy their energy demands, so there has to be a steady influx into the colony. Our model models these processes described above. Each single agent (bee) can switch from task to another with a probability that changes over time, this can lead to specialisation.. We implemented a self-reinforcement mechanism that showed interesting properties: It keeps the plasticity of the systems in times of perturbations, but makes the workers specialise on one task in times when the system is at equilibrium state. Our agents can emit stimuli (dances, chemical signals) that are found with real bees. This is important, as one of our main goals was to see how our model of self-organised division of labour works with these nature-near types of stimuli.

Using our model, we could successfully repeat empirical experiments performed with real bees. We investigated the role of the heterogeneity of the environment in the task selection process and we could show how brood nursing is performed in a decentralised homeostatic way in a honeybee colony.

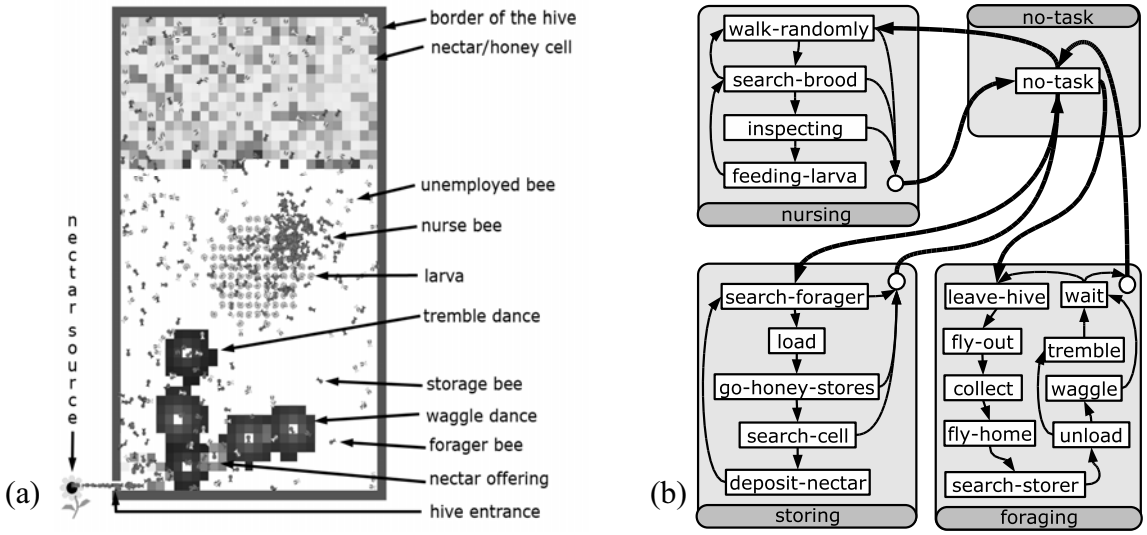


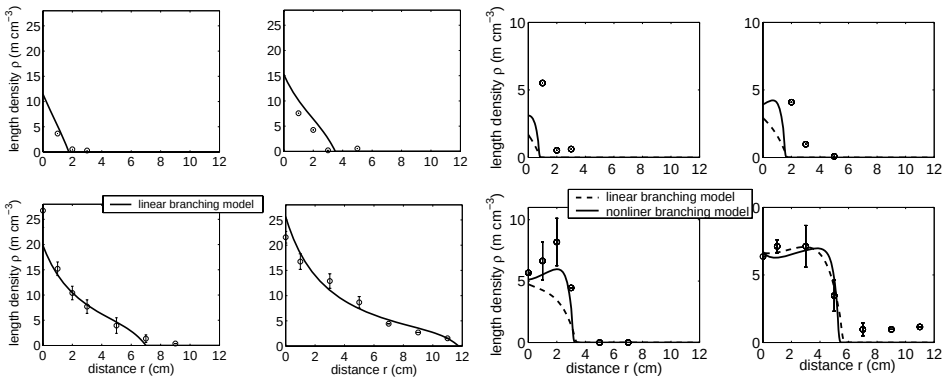
Figure 1: (A) A screenshot of our simulation at runtime. (B) Within each single individual bee (agent) shown on the left sub-picture, a finite state automaton works (=behaviour).

GROWTH MODEL FOR MYCORRHIZAL FUNGI

A. Schnepf[1,2] and T. Roose[2]

Corresponding Author: A. Schnepf
[1]BOKU-University of Natural Resources and Applied Life Sciences
Department of Water, Atmosphere and Environment
Muthgasse 18, 1190 Vienna, Austria
Phone: + 43 1 36006-5482, Fax: + 43 1 36006-5499
Email: andrea.schnepf@boku.ac.at
[2]University of Oxford, Mathematical Institute
Oxford Centre for Industrial and Applied Mathematics and Centre for Mathematical Biology
24 - 29 St. Giles, Oxford OX1 3LB, UK

Arbuscular mycorrhizas are mutualistic symbiotic associations between plant roots and soil fungi. They are thought to provide plants with an enormous spatial advantage to access nutrients of low mobility from the soil, *e.g.* phosphorus. We extend the fungal growth model of [1] by using time dependent boundary conditions that describes the dynamics of hyphal tips at the root surface. The experimental data of [2] are used for model calibration and for deriving fungal growth parameters. Good agreement is



(a) *Scutelospora calospora* (b) *Glomus sp.*

Figure 1: Solution of the linear and nonlinear branching model in comparison to data of [2]. See the full paper for model equations and parameter values.

found between the linear branching model and the measured hyphal length densities of the fungal species *Scutelospora calospora* (see figure 1(a)). For this fungus, the colony growth appears to be dominated by the root infection rate rather than tip branching rate. For *Glomus sp.*, we modify the model to include the effect that there might be a maximal hyphal tip density after which no branching takes place. The results for this fungus are shown in figure 1(b).

Thus, we conclude that our model is applicable to mycorrhizal fungi. However, it is necessary to adapt it carefully for individual fungal species. Results of this paper give us confidence to use the fungal growth models presented here for computing mycorrhizal nutrient uptake.

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TIME DELAY MODEL OF ALGAL POPULATION GROWTH IN A PHOTOBIOREACTOR

J. Fišer, J. Červený and P. Zítek, CTU in Prague, Czech Republic

Corresponding Author: J. Fišer,
Centre for Applied Cybernetics
Czech Technical University in Prague
Technická 4, 166 27 Praha 6, Czech Republic
Phone: +420 22435 3953, Fax: + 420 23333 5604
e-mail: Jaromir.Fiser@fs.cvut.cz

There are two basic reasons why delays become a natural phenomenon in dynamical development of biological systems, referred to as population growth models [5]. The time delays are usually introduced rather qualitatively in common population models but their application to particular bioreactor technology is dealt with only scarcely [2]. A widely applied population growth model has been developed on the basis of delayed Volterra-Lotka equations [2] while a more specific model respecting the age relationships can be found in [3]. A consistent survey of modelling algae culture growth can be found in [4].

A basic objective of a continuously operating photobioreactor is to aim at a constant rate of population growth, also referred to as balanced growth rate. To reach the balanced growth rate the following prerequisites are to be provided: continuous food supply, sufficient and least variable lighting and steady environmental parameters in algae cultures [1]. Data acquisition from the algae biomass production needed for the model formulation consists of the measurement of incident light intensity, water medium temperature and off-line measurements of dry weight of algae.

For the purposes of modelling the tubular photobioreactor technology a novel model structure is proposed in the paper. It is based on the delayed Volterra-Lotka equation population model with aditional functional terms expressing the influence of age distribution on population growth in following form

$$\frac{dx(t)}{dt} = \left[\mu(x, I, \vartheta) - \int_0^T dA(\tau) x(t-\tau) + \rho \int_0^T dB(\tau) \frac{dx(t-\tau)}{dt} - m(x, I, \vartheta) \right] x(t-d) \tag{1}$$

where $A(\tau), B(\tau)$ are functions of delay distribution defined on the interval $\tau \in \langle 0, T \rangle$, T is the largest delay length, μ and m are the specific rate of growth and mortality rate, ρ is to distinguish the different levels of food consumption in a growing and mature populations. The distribution functions $A(\tau), B(\tau)$ are positive over the entire interval of τ. While $A(\tau)$ refers to the bounded space for the culture growth the distribution $B(\tau)$ expresses the influence of the ageing part of the population on the growth.

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OBJECT ORIENTED MODELLING OF METABOLIC PATHWAYS

A. Belič[1], R, Karba[1], K. Fon-Tacer[2], T. Režen[2], D. Rozman[2]

[1]Faculty of Electrical Engineering, University of Ljubljana

[2] Center for Functional Genomics and Bio-Chips
Institute of Biochemistry, Faculty of Medicine University of Ljubljana

Corresponding author: A. Belič
Faculty of Electrical Engineering
University of Ljubljana
Tržaška 25, SI-1000 Ljubljana, Slovenia
Phone: +386 1 4768 762, Fax: +386 1 4264 631
ales.belic@fe.uni-lj.si

Mathematical modelling of metabolic processes has a long history. Mostly, compartment-type models were used to describe the metabolic networks. However, up till genome project, metabolic networks were rather small. Classical pharmacokinetics used compartmental models with up to three compartments. Later-on the number of compartments was enlarged, as analytical methods were capable of detecting more detailed dynamics of the system. One of the major problems of multi-compartment models was the identifiability of their parameters, as measurements were in most cases made for the quantities in only few compartments. The next problem arose due to non-exact understanding of metabolic pathways. Therefore, it was necessary to simplify the model structure, reducing the model to a dynamical model whose structure could only vaguely be compared with the real system's structure. Identification of the smallest possible structure with respect to the measurements is the only feasible procedure. Functional genomics, however, has started producing enormous quantities of data, and practically each chemical reaction in the metabolic pathway has been monitored. Therefore, large multi-compartment models can be composed and their parameters are directly related to the specific chemical reactions. The procedures of modelling must therefore be altered to address the problem of handling such large models. Graphical representations, as are offered by MATLAB/SIMULINK, are very effective for classical compartment-type models, however, when dealing with hundreds of compartments, block diagrams become very ineffective. Each compartment must be modelled uniquely, and due to large number of blocks and connections the SIMULINK scheme becomes unclear. Any changes of the model become very tedious and prone to mistakes. Usage of object oriented tools offers better solutions, however, the definition of objects of the system must be made according to the system's structure. In the present article, object oriented modelling of cholesterol metabolic pathway, using Modelica standard language for object oriented modelling is shown in compare with SIMULINK. The cholesterol metabolic pathway model is being developed for the STEROLTALK 6th EU framework project. The modelling aim is to construct a model that will provide better insight into cholesterol metabolic pathways, and thus, to improve hyper-cholesteremia treatment. The composition of the model in Modelica standard shows significant advantages over SIMULINK realisation. The Modelica version, due to object oriented approach is more transparent, and any changes to the model are easier. Block oriented approach is not feasible for the construction of metabolic pathway models. However, Dymola lacks the tools for simulation results analysis, where MATLAB/SIMULINK shows obvious advantage. The solution, which is also supported by the Dynasim is in the combination of the two environments. From the modeller's point of view it is still a bit awkward solution, since one is still forced to use both tools. The optimal solution would still be in one complete modelling environment. On the other hand, the combination of both tools provides a means for simulation validation, especially in the case of cholesterol, where the system is complex and non-linear. Although the text version Modelica model is more transparent than SIMULINK version of the model, graphical representation of the models in Modelica library will have to be implemented. The reason is twofold: transparent structure for the modeller and easier communication with problem scientists. Current cholesterol model is in the very early stage of model development and the simulation results have no significant biological meaning. However, the work that has been done till now shows possible problems that will arise during model development and indicates possible workarounds.

THE TOTAL QUASI-STEADY STATE APPROXIMATION FOR COMPLEX ENZYME REACTIONS

M. G. Pedersen, Technical University of Denmark, Kgs. Lyngby, Denmark
A. M. Bersani, University "La Sapienza", Rome, Italy
E. Bersani, Datalink Informatica, Rome, Italy
G. Cortese, University of Padova, Italy

Corresponding Author: A.M. Bersani
University "La Sapienza"
Dept. of Mathematical Methods and Models (Me.Mo.Mat.)
Via A. Scarpa 16, 00161 Rome, Italy
Phone: +39 0649766681, Fax: +39 0649766684
email: bersani@dmmm.uniroma1.it

Abstract. Biochemistry in general and enzyme kinetics in particular have been heavily influenced by the model of biochemical reactions known as Michaelis-Menten kinetics [3]. This formulation considers a reaction where a substrate S binds reversibly to an enzyme E to form a complex C. The complex can decay irreversibly to a product P and the enzyme, which is then free to bind another substrate molecule. Assuming that the complex concentration is approximately constant after a short transient phase leads to the usual Michaelis-Menten (MM) approximation (or *standard quasi steady-state approximation* (sQSSA)), which is valid when the enzyme concentration is sufficiently small [5], [6]. This condition is usually fulfilled for *in vitro* experiments, but often breaks down *in vivo*.
The total QSSA (tQSSA) [2], which is valid for a broader range of parameters covering both high and low enzyme concentrations, has been introduced in the last two decades. Tzafriri [7] showed that the tQSSA is at least roughly valid for any set of parameters.
This newer approximation has so far only been applied to isolated reactions. However, *in vivo* the reactions are coupled in complex networks or cascades of intermediate, second messengers with successive reactions, competition between substrates, feedback loops etc. Approximations of such scenarios have been carried out within the MM scheme [1], but often without a thorough investigation of the validity of the approximations. An exception is the case of fully competitive reactions [4], [5], i.e., reactions with competing substrates, also known as substrate-inhibitor systems. However, since the MM approximation cannot be expected to be valid *in vivo*, employing the tQSSA to these more complex situations would be beneficial.
We extend the tQSSA to more complex reaction schemes, like fully competitive reactions, double phosphorylation, Goldbeter-Koshland switch and we show that for a very large range of parameters our tQSSA provides excellent fitting to the solutions of the full system, better than the sQSSA and the single reaction tQSSA.
Finally we discuss the need for a correct model formulation when doing "reverse engineering". We show that estimated parameters are much closer to the real values when using the tQSSA that the sQSSA, which can even overestimate the parameter values greatly.

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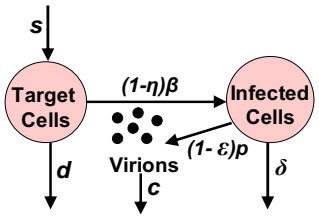
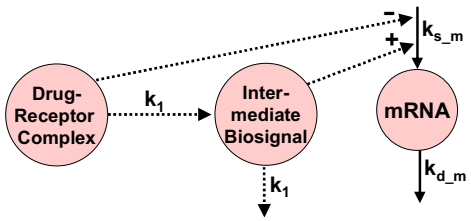
MODELING THE DYNAMICS OF BIOCONTROL SYSTEMS MECHANISTICALLY

R.M. Javier and J.J. DiStefano III, UCLA, Los Angeles, CA, USA

Corresponding Author: R.M. Javier
5123 Keynote St, Long Beach, CA 90808
Phone: 1-562-760-5299, Fax: 1-562-420-9109, Email: neurobyn@ucla.edu

Mathematical models and systems biology methods are used to describe numerous biological systems, with an overall goal of providing new levels of descriptive and predictive power. The specific modeling approach, of course, varies in accordance with the particular goals of the modeler. Many models are necessarily or decidedly *macroscopic*, i.e. their components aggregate lower level, more *microscopic* details typically insufficiently well-known. They usually capture essential or overall dynamics rather than minute or microscopically detailed behavior. The various predator-prey models of HIV and hepatitis-C virus (HCV) [7] dynamics of the Perelson group, for example (shown.), have been necessarily quite macroscopic, because little was known about the detailed mechanisms involved, and this is still the case. Nevertheless, they captured pertinent dynamics of these disease processes in the whole organism, under treatment with antiviral drugs over the scale of days or weeks. To understand the control *mechanisms* involved in biocontrol processes, a more microscopic and usually molecular level approach usually is required. To address intra- and intercellular control, and mechanisms of action of bioactive substances, e.g. protein signaling and intracellular signal transduction, one must model the intracellular processes and couplings among these signals. Since models at this level of detail are typically based in physiology and biochemistry, and not simply generalized equations, their construction requires significantly more information about molecular network topologies, details which unfortunately are often uncertain or incomplete. However, this apparent obstacle is also the biggest advantage in using such models, namely the power to elucidate mechanisms through an iterative process of model construction and comparison with data, i.e. a mechanistic model of a system can be proposed as a hypothesis to be supported or refuted by experimental observations. In this way, we can glean a better understanding of how a system is or is not put together, morphologically and dynamically.





We examine some representative examples of more or less mechanistic approaches, illustrating ways various investigators handle data-driven modeling problems associated with drug effects on the whole organism [7], switch-like responses in cell signaling subsystems [2], gene network regulation [4] (shown) and tumor-suppressor protein regulation mechanisms [1,3,5,6]. These distinct biosystems and model representations demonstrate to varying degrees the power of more microscopic methods for testing and sorting through alternative mechanistic hypotheses.

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IDENTIFIABLE REDUCED COMPLEXITY MODEL FOR THE HUMAN RESPIRATORY AND CARDIOVASCULAR SYSTEM

M. Hirsch, C. Furtmueller and L. del Re, Johannes Kepler University Linz, Austria

Corresponding Author: M. Hirsch
Johannes Kepler University Linz
Institute for Design and Control of Mechatronical Systems
Altenbergerstraße 69, 4040 Linz, Austria
Phone: +43 732 2468- 9773, Fax: +43 732 2468- 9759
email: markus_hirsch@gmx.at

Abstract. There exist several mathematical models of the human body during exercise as presented for example in [4] and [5]. Even models which contain the periodicity of breathing, like the one presented by Grodins [2], have been developed. Most of them are highly complex and contain several unknown parameters, which however cannot be easily identified from non invasive measurements. The aim of this work is to propose a model of the cardiovascular and respiratory system of reduced complexity which captures the central characteristics of the system and can be parameterized using simple measurements. This paper starts with deriving a reduced complexity model from the model proposed by Batzel [1] and Khoo [3]. An ergometer is then used to gather measurement data of a test person and to use this to identify the model parameters. The parameterized model was then implemented to simulate the behavior of the human body under aerobic exercise. Comparisons between measurements and computed values confirm the validity of the approach.

Prospect

There are many reasons to simulate complex processes of the human body, as for analyzing and treating diseases, evaluation of the training status in sports, medication and in general to analyze physiological control systems.

In this work the interesting and highly complex process of the energy supply is treated. Normally models for the simulation of the human respiratory and cardiovascular system are very complex such that identification with easily measurable data is not possible. Often however such identification is the basis of any analyses tasks. This work presents a way to analyze such complex processes by reducing the model to the significant effects, such that identification is possible.

Further a short description of the way regulation of ventilation and blood flow works is presented. Understanding this behavior a model is build up, which is very simply and elementary in structure such that identification with no invasive measurement data can be done. The measured data consists of four signals: The input signal of the system which is presented by the physical load a human is bringing up on an ergometer and three output signals, the heart rate, the airflow of the inhaled air and the concentration of carbon dioxide of the exhaled air.

By pre-processing the data, the effects of periodic breathing have been eliminated and average signals for blood flow, ventilation airflow and partial pressure of carbon dioxide in arterial blood have been obtained. Then this data has been used directly to identify the reduced complexity model.

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Hemodynamic Models for Education in Physiology

M. Hessinger, A. Holzinger, MedUni Graz, Austria
D. Leitner, TU Vienna, Austria
S. Wassertheurer, ARCS, Austria

Corresponding Author: S. Wassertheurer
ARC Seibersdorf research GmbH
Florag. 7/407, 1040 Wien, Austria
Phone: +43 1 58801-10143, Fax: + 43 1 58801- 10195
email: siegfried.wassertheurer@arcsmed.at

Abstract
By application of Case-Based Learning (CBL) various effects can be analyzed and demonstrated more easily. In the area of medicine one rapidly reaches boundaries in the visualization of complex information[1]. Learning and teaching without recourse to patients is difficult. Consequently the use of models and simulations are useful in this respect. In this paper the authors report about experiences gained with HAEMOSIM, a web based project in medical education. The goal of this project was the design and development of interactive simulations in local hemodynamics by the application of mathematical-physiological models. These include the modeling of arterial blood flow dependent on the pressure gradient, radius and bifurcations, as well as blood flow profiles in dependency of viscosity, density and radius and finally pulse-wave-dynamics with regard to local and global compliance.

Concept
Unlike most technical applications human bloodfow is unsteady and the tubes are compliant. Furthermore the investigator has to consider reflected and rereflected pressure waves too. Out of this, the current work aims to provide web based simulation models to give a stepwise and interactive introduction to steady and unsteady pressure and flow relations in compliant tubes. The learning structure is organised in the sections 'Basic laws for steady flow in tubes' ,'Unsteady (pulsatile) flow in straight elastic tubes under homeostatic conditions' and ' Transient bloodflow in arteries'. Within each step we introduce new concepts and its limits. This subsequently leads to the next level.

Modelling and Simulation
Within the medical domain blood pressure is one of the most popular forces. Pressure is defined as force per area and popular measuring units are mmHg or dyne/cm². Force itself can be defined for our purposes as accelerated mass, what subsequently implies that there is the necessity of kinetic energy to produce pressure. Based on this both Hagen and Poiseuille indepently started to investigate the behaviour of flow in small rigid tubes. Finally Poiseuille found a formular which explains that flow in the desired pipes is subject to the pressure difference (δP), pipe length (L), pipe radius (R) and fluid properties like viscosity and density [2]. Unfortunately the law of Hagen-Poiseuille can't fully applied to the human cardio-vascular system. Nevertheless the law of Hagen-Poiseuille is a fundamental basis and delivers qualitative insight to flow in tubes. To provide further insight we developed additional applications. For considering elasticity we introduce both the concept of compliance and elastic (Young) modulus as well as the resulting pulse wave velocity. To overcome the steadiness we present an analytic solution to the linearized Navier-Stokes equations in frequency domain based on Womersley[3]. Finally we consider the full fluid mechanical model using a Lattice-Boltzmann Model which is proven to converge against the Navier-Stokes equations[4,5].

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EVALUATION OF RUPTURE OF INTRACRANIAL SACCULAR ANEURYSMS BASING ON THE MODEL USING LEGENDRE FUNCTIONS

K.Szafrański, TU Szczecin, Poland

Corresponding Author: K.Szafrański
Szczecin University of Technology
Ul. 26 Kwietnia 10, 71-126 Szczecin, Poland
Phone: +48 91 4523-622 or +48 607 333-105
email: kris790@wp.pl

One of the main problems in the contemporary medicine is predictiion of rupture of intracranial saccular aneurysm. According to the previous tests and researches the main focus was to find critical relationships based on the maximal dimension of an aneurysm. Studies on unruptured intracranial aneurysms proved that the size is not the proper predictor of risk of ruptures in lesions of diameter less than 10 mm [1], as Weibers concluded. Finally, the scientists came to the point, that shape of an aneurysm should be analysed carefully, and that modelling should be performed by the means of more complicated shapes [3]. The shape (curvature) can be the valuable predictor for the calculation of stresses. The curvatures have already been calculated basing on the boundary points, which defined the surface of the aneurysm. These points allowed for the interpolation of remaining points on the surface and calculation of specific points for shape of an aneurysm. The use of splines and a special procedure within a solid-modelling package, IDEAS, made it possible to create three-dimensional reconstructed surfaces, and then the splines were used to calculate the local curvatures. This method of calculation of curvatures proved to be time-consuming (order of ten hours) and is rather impractical for online testing of the patient undergoing CT or MRI.

Therefore I decided to make researches in order to apply suitable mathematical functions for the model of an intracranial saccular aneurysm.
Following the detailed analysis of shape of an intracranial aneurysm I have decided to choose the Legendre functions for modelling.
The shape of an aneurysm can be described as follows:

$$r = \beta(1 + c \cdot P_n^m(\cos\phi) \cdot \cos(m\theta)) \tag{1}$$

The above formula includes the following parameters: r is the radius, ϕ is from [0,π] and θ is from [0,2π]. ϕ and θ are angles in spherical coordinates, P_n^m is the Legendre function of the first kind, and β, c, n and m are shape parameters. The shape can be defined for any value of ϕ and θ, if the center point and the equation for radius are determined.
Moreover, I have minimised the difference between the actual radius of the aneurysm and radius of the aneurysm modelled by using the Legendre functions. The sum of the square errors was minimised thanks to the Marquardt-Levenberg regression code. The standard Legendre functions decreased RMS values for five exemplary aneurysms of about 40 % in comparison to models based on the sphere. The modification of the standard Legendre functions by the scalar multiplies improved these results by about 10 %.
Another main point of this paper is calculation of the curvatures [2]. Calculations are performed in Matlab, while curvature maps are presented in Maple. The curvatures were calculated as the maximal and minimal values of K_n known as the normal curvature and strictly related to the curvature vector k. The impact of the perpendicular component of the curvature vector was not taken into account.
The maximal (η_1) and minimal (η_2) values of the normal curvature were received upon calculation of $dK_n/d\lambda=0$ and finally stresses were obtained in relation to the maximal and minimal curvatures. The researches proved that stress resultants could be calculated independent of the properties of the material and knowledge of the principal curvatures.

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Mathematical Modelling and Control of Chemical and Biochemical Processes

DESIGN OF ESTIMATORS FOR SPECIFIC GROWTH RATE CONTROL IN A FED-BATCH *E. COLI* FERMENTATION

I. Rocha[1], A. C. A. Veloso[1,2] and E. C. Ferreira[1]
[1] Centro de Engenharia Biológica, Universidade do Minho, Braga, Portugal
[2] Escola Superior Agrária de Bragança, Bragança, Portugal

Corresponding Author: E. C. Ferreira
Centro de Engenharia Biológica
Universidade do Minho
Campus de Gualtar – 4710-057 Braga, Portugal
Phone: +351 253 604400, Fax: + 351 253 678986
email: eugenio@deb.uminho.pt

The specific growth rate is one of the most important process variables characterizing the state of microorganisms during fermentations mainly because the biosynthesis of many products of interest is often related with the values assumed by this parameter. In the particular case of the fed-batch operation of *Escherichia coli* for the production of recombinant proteins, it is important to maintain the specific growth rate below a certain threshold in order to avoid the accumulation of acetic acid throughout the fermentation and, additionally, it is often argued that both pre- and the post-induction specific growth rates should be closely controlled in order to achieve maximum productivities on the desired recombinant protein.

The main purpose of this work was to develop reliable algorithms for the estimation of the specific growth rates in *E. coli* fermentation that can be used for the feedback control of this variable using a developed mathematical model of the process, together with on-line measurements commonly available both in research labs and in industry.

For that purpose, a biomass asymptotic observer is derived for the on-line estimation of biomass concentration. Using estimated biomass concentration values, together with on-line process data, the determination of the specific growth rates is performed using observer-based estimators. Finally, a feedback-feedforward control algorithm was developed that uses estimated values of the specific growth rates and biomass for the calculation of the feeding rate. The developed algorithms were validated by simulations where on-line variables used for the calculation of the estimators were corrupted with white noise.

With the these algorithms, it was possible to estimate with great accuracy the specific growth rates and biomass concentration during a recombinant *E. coli* fermentation using on-line data from dissolved oxygen and carbon dioxide, oxygen and carbon dioxide transfer rates and culture weight. The feedback-feedforward controller was able to keep the specific growth rate at the desired setpoint even in the presence of perturbations both in the model parameters and in the concentration of substrate in the feeding solution.

Future work involves the implementation of a more rational tuning procedure, including the optimization of tuning parameters by minimizing the differences between the desired setpoint and the real specific growth rates and also the experimental validation of the algorithms.

FROM OPTIMAL TO PRACTICALLY FEASIBLE TEMPERATURE CONTROL OF A TUBULAR REACTOR

F. Logist[1], I.Y. Smets and J.F. Van Impe, K.U.Leuven, Belgium

Corresponding Author: J.F. Van Impe
BioTeC - Katholieke Universiteit Leuven
W. de Croylaan 46, 3001 Leuven, Belgium
Phone: +32-16-32.14.66, Fax: + 32-16-32.29.91
email: jan.vanimpe@cit.kuleuven.be

Due to market saturation and global competition, today's chemical industry strives for more efficient processes to reduce the production costs. Mathematical process models and computers have proven over the past decades to be extremely valuable tools for optimizing the design and the operation of chemical processes, resulting in the desired profit improvement. Application of these model based techniques to tubular reactors, still important workhorses in the process industry, opens the door to improved design and operation policies [2].

In this paper the optimal steady-state control of a jacketed tubular reactor is studied. Therefore, the problem is cast into the framework of *optimal control theory* (also called *dynamic optimization*). Both *analytical* (Pontryagin's minimum principle, see, e.g., [1,3]) and *numerical* techniques (control vector parameterization, see, e.g., [4,5]) are combined in order to compensate for their weaknesses while enhancing their strengths. To obtain optimal temperature profiles along the reactor, which are feasible to implement in practice, (i.e., without discontinuities requiring an infinite heat transfer rate), not the reactor temperature itself, but the heat flux between the reactor and the jacket is selected as the control variable. This heat flux is then related to the gradient of the (dimensionless) reactor temperature in order to allow an easier physical interpretation.

To measure the reactor performance both *conversion* and *energy* costs are taken into account. Two cost criteria are studied, i.e., one consisting of only terminal cost terms and a second one combining a terminal and an integral cost part. During each optimization great care is taken to ensure a *safe* operation by limiting the reactor temperature.

Several generic features of the resulting optimal profiles are recognized and interpreted based on the terms in the cost criterion, yielding additional insight into the process. For the terminal cost criterion it is important to keep the temperature as high as possible in the first part of the reactor (without violating the maximum temperature constraint) in order to favor conversion. In the second part, however, cooling is required to reduce the terminal heat loss. For the terminal and integral cost criterion, the temperature is first brought to an intermediate level and kept constant in order to reduce the global heat loss and the chance of the occurrence of hot spots, while in the second part an additional temperature rise induces additional conversion of reactant. In addition, the effect of the maximum reactor temperature constraint is illustrated. Without a temperature limit, higher reactor temperatures, which favor conversion, are observed, resulting in a lower optimal cost value for both criteria.

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MODELLING THE RESPONSE OF THE MARINE MICRO ALGAE *EMILIANIA HUXLEYI* TO AN ELEVATION OF pCO_2

O. Bernard, S. Madani and A.Sciandra

Corresponding Author: O.Bernard
COMORE (Modelling and Control of renewable Resources)
INRIA, BP 93,06 902 Sophia-Antipolis cedex, France
Phone: +33 492 387 785, Fax: +33 492 387 858
email: olivier.bernard@inria.fr

Coccolithophorids are marine microalgae producing micro calcite plates. Under certain circonstances these microorganisms can form massive blooms which can be detected by satellites. These phytoplanktonic organisms play an important role in atmospheric CO_2 trapping through large scale precipitations of calcium carbonate in the oceans.

However, recent experiments revealed that the associated fluxes that represent a sink of carbon may be slow down by an increase in atmospheric CO_2 concentration. In this paper we design models to account for the decrease in calcification and photosynthesis rates observed after an increase of pCO_2 in *Emiliania huxleyi* continuous photobioreactors. Since the involved mechanisms are still not completely clear, we developed several models, each of them based on a different hypothesis. These models are kept at a very general level, by maintaining the growth and calcification functions in a generic form, *i.e.* independent on the shape of these functions and on parameters values. The mathematical analysis of the models at steady state is thus performed using these generic functions were the only hypothesis is an increase of these rates with respect to the regulating carbon species. As a result, each model responds differently to a pCO_2 elevation. Surprisingly, the only model whose behaviour is in agreement with the experimental results corresponds to a coupling of photosynthesis and calcification with carbonate as the regulating species, whereas bicarbonate is the substrate of these processes.

Left: *Emiliania huxleyi*. Right: bloom of E.huxleyi detected from satellite (south of Cornwall, UK).

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Metabolic Flux Analysis : an approach for solving non-stationary under-determined systems

A. Provost and G.Bastin

Cesame, Université Catholique de Louvain
av. Georges Lemaître 4, 1348 Louvain-la-Neuve, Belgium
Phone:+32 10 478032 Fax: +32 10 47 21 80
email: (provost, bastin)@auto.ucl.ac.be

We consider a cell line cultivated in batch mode in a stirred tank reactor. From a macroscopic viewpoint, the cell mass in the reactor is regarded as a device that catalyses the conversion of substrates into products. The dynamics of the substrates and products are described by the classical differential equations

$$\dot{s} = -v_s X \tag{1}$$
$$\dot{p} = v_p X \tag{2}$$

whith X the biomass concentration, s the vector of substrate concentrations in the reactor, p the vector of product concentrations, v_s the vector of specific uptake rates and v_p the vector of specific excretion rates.
Obviously the specific rates v_s and v_p are not independent : they are quantitatively related through the intracellular metabolism represented by a metabolic network that encodes the set of reactions which take place within the cell. In the graph of the network, the nodes represent the internal metabolites and the edges represent the metabolic fluxes. According to the fundamental quasi-steady state assumption of Metabolic Flux Analysis (MFA), it is assumed that, for each internal metabolite, the net balance of production and consumption fluxes is equilibrated. This is expressed by an algebraic relation

$$Nv = 0 \tag{3}$$

where v is the vector of fluxes v_i and $N = [n_{ij}]$ is the stoichiometric matrix of the metabolic system.
By definition, the specific rates v_s and v_p are linear combinations of some of the metabolic fluxes. This is expressed by defining appropriate matrices N_s and N_p such that

$$v_s = N_s v \qquad v_p = N_p v. \tag{4}$$

The purpose of "Metabolic Flux Analysis (MFA)" is to compute the unknown flux distribution (i.e. the vector v) from measurements of the specific rates v_s and v_p. The goal is thus to find a non-negative solution to the linear system

$$\begin{pmatrix} N \\ N_s \\ N_p \end{pmatrix} v = \begin{pmatrix} 0 \\ v_s \\ v_p \end{pmatrix} \tag{5}$$

Our concern in this paper is to perform the MFA all along the cell life. The problem faces two basic difficulties. First the system (5) is usually under-determined : there are more unknowns than equations. And secondly the metabolic routes within the cell can change during the cell life in a way which is in particular related to the availability of the substrates. This means that the structure of the matrix N itself can change.
In order to account for the changes of the metabolism we consider three successive metabolic networks corresponding to the three successive typical phases during the cell life, namely the growth phase, the "plateau" phase and the death phase.
Then, for each network successively, in order to solve the under-determination problem, we compute the "Elementary Flux Modes (EFM)" that connect the substrates to the products. The flux distribution is described as a combination of Elementary Flux Modes. The admissible weights of this combination are given by the entries of a vector that solves a problem derived from the MFA problem (5).
Finally, a complete MFA is obtained by using the three separate models in their respective time interval, smoothly switching from model to model on the basis of the availability of the substrates.
The methodology is illustrated with experimental data of CHO cell batch cultivations.

MECHANISTIC KLA MODELLING IN AN UPFLOW ANAEROBIC DIGESTER

J.Hess and O. Bernard, INRIA, France

Corresponding Author: J.Hess
COMORE, INRIA
BP 93, 06902 Sophia-Antipolis cedex, France
email: jonathan.hess@inria.fr

Anaerobic digestion is a wastewater treatment process involving bacteria to degrade polluting organic matter and transform it into CO_2 and methane (CH_4). This process can therefore be used for organic pollution removing or for renewable energy production, thanks to cogeneration of methane leading both to electricity and/or heat. However, a constant ratio of CO_2 and CH_4 is crucial to guaranty an optimal yield of methane use. A modelling step is thus required, in order to better control and exploit the produced biogas whose quality is known to be largely variable. The anaerobic digestion process is however very complex from a biological point of view as it can involve hundreds of microorganism species, is non linear and can adapt to new environmental conditions. This system is also complex even from a physical point of view since it involves three different phases: liquid (dissolved compounds), solid (biomass, flocks or bacterial bed) and gaseous (bubbles that are rising in the digester). The physical interactions of these phases may deeply impact the processes, and it plays a crucial role on the liquid-gas transfer coefficient K_La. This coefficient is defined as the product between the transfer coefficient K_L and the surface of exchange a between the two phases. The surface is mainly defined by the surface of the bubbles in the reactor. We propose here a model that details the mechanism of bubble nucleation and bubble rise in the digester. The model assumes that after bubble nucleation, CO_2 is incorporated into the bubble during its ascension. The total flow of methane and CO_2 in the bubbles is then computed depending on the dissolved CO_2 and on the methane production rate, assumed to be homogeneous in the digester. The apparent K_La deduced from the resulting total CO_2 flow rate can then be estimated and related to the dissolved CO_2. It turns out to be an increasing function of the methane and CO_2 flow rates. This crude mechanistic model can then be used to derive a simple reduced model for the K_La and thus contribute to improve biogas quality predictions.

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PDAE Models in Engineering Applications

MODELING WITH PARTIAL DIFFERENTIAL-ALGEBRAIC SYSTEMS IN CHIP-DESIGN

A. Bartel and R. Pulch, BU Wuppertal, Germany

Corresponding Author: Andreas Bartel
Lst. Angewandte Mathematik/Numerische Analysis
Bergische Universität Wuppertal
D-42097 Wuppertal, Germany
bartel@math.uni-wuppertal.de

The usual modeling of electric circuits yields systems of time-dependent differential-algebraic equations (DAEs). Due to down-scaling, secondary effects become more and more important: that is, for instance, thermal-conduction, transmission line phenomena or complex semiconductor behavior. Here more sophisticated models enrich the DAE by spatial systems, which results in a partial differential-algebraic equation (PDAE) depending on both space and time. Furthermore, the system of DAEs may exhibit a multirate behavior purely in time with an oscillatory fast time scale. Here a multidimensional signal model yields PDAEs depending on different time scales.

In both cases, the PDAE-model gives us an adequate and versatile description of the underlying physical behavior to study and simulate electric networks. We distinguish three classes of models:

1) Refined networks (transmission line/semiconductor): Network elements are replace by a PDE-description. Boundary conditions (PDE) are determined from the node potentials, and PDE-currents serve as source for the electric network. In this way, it is possible to show that drift-diffusion coupled with electric networks permit unique solutions of the underlying PDAE (semiconductor case). Furthermore, for transmission lines we have hyperbolic equations, such that upwind schemes are proven to be robust and efficient.

$$\tfrac{\mathrm{d}}{\mathrm{dt}} q(u) = f(u,T) + s(t) + A_S\lambda, \qquad M_S\partial_t\phi = \mathcal{L}(\phi), \quad \mathrm{BC}(\phi) = A_S^\top u, \quad \lambda = \mathcal{P}(\phi).$$

2) Multiphysics (heat conduction): Parameters of the electric network depend on temperature. Therefore it is in general not possible to have refined networks, but one has a special geometry. For SOI chip-design an accompanying thermal network (AN) consisting of 0D and 1D elements is proven to be adequate (permits unique solutions). Furthermore, a multirate algorithm has been successfully designed and applied to industrial benchmarks.

$$\tfrac{\mathrm{d}}{\mathrm{dt}} q(u) = f(u,T) + s(t) \qquad M\partial_t T = \mathcal{L}(T) + P(u)$$

3) Multitone extension (two-tone quasiperiodic): The electric circuit exhibits oscillations in well-separated frequencies. Introducing according time variables, the network DAE transforms to a hyperbolic PDAE, where the integration process is now confined to the rectangle of periodicities. This enables an adequate representation of the multitone signal, and an efficient solution strategy via a method of characteristics.

$$\tfrac{\partial}{\partial t_1} q(\widehat{u}) + \tfrac{\partial}{\partial t_2} q(\widehat{u}) = f(\widehat{u}) + s(t_1, t_2)$$

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Modeling and Simulation of Shape Memory Behavior

G. Teichelmann and B. Simeon, Munich University of Technology, Germany
D. Helm, University of Kassel, Germany

Corresponding author: Gunnar Teichelmann,
TU München, Zentrum Mathematik, M2
Boltzmannstraße 3, 85748 Garching, Germany
email: teichelmann@ma.tum.de

Shape Memory Alloy (SMA) materials have an enormous potential in technological applications like aviation or medicine among others. In robotics they can be used as temperature controlled actuators and allow the design of quite small manipulators. Here the material model described in [1] will be used, that is able to reproduce the main phenomenological aspects of shape memory behavior like one- and two-way effects as well as pseudoelasticity and pseudoplasticity.
A material point x in referential coordinates is mapped to its position on the deformed domain by the deformation function $\vartheta(t,x) = x+u(t,x)$ with the displacement field u. We formulate the quasistationary momentum balance $0 = \text{div } \sigma(t,x) + \beta(t,x)$ with the symmetric stress tensor σ and the density of body forces β. Furthermore, we have mixed Dirichlet and Neumann boundary conditions and of course consistent initial conditions. The kinematic relation between displacement u and strain ϵ is represented by the linearized Lagrangian strain, while the total strain is decomposed by $\epsilon = \epsilon_\text{p} + \epsilon_e$ into plastic and elastic strain. The relation between stress σ and elastic strain ϵ_e is then given by a generalized Hooke's law, depending also on the temperature. There are 6 ways for the volume fractions of temperature induced martensite z_TIM, stress induced martensite and austenite to change from one to another. The decision which transition is active depends mainly on the temperature and its rate, the martensite fractions, the loading conditions, the internal stress X and the value of the yield function

$$\Upsilon(\sigma,\theta,X) = ||\sigma - X|| - \sqrt{\frac{2}{3}}k(\theta),$$

that resembles the viscoplastic case. The variables z_TIM, X and ϵ_p are internal values, that are incorporated by evolution equations, whose right hand sides discontinuously depend on the actual phase transition. Now the heat equation has to be introduced, adapted to the deformed domain. Hence using differential geometry methods [2] and introducing a geometrical parameter ζ we arrive at

$$\rho_0 c_0\, \theta_t = -\frac{\lambda\, u_{xx}}{\zeta(1+u_x)^2}\cdot\theta_x + \frac{\lambda}{\zeta(1+u_x)}\cdot\theta_{xx} + \frac{1+u_x}{\zeta}\, f, \quad x\in\Omega,$$

where the source term $f(t,x)$ depends on all the variables and their change rates in time.
For solution purpose we first use a finite element approach for semidiscretization in space of the quasistationary momentum balance and the heat equation. In this course the discretization points of the internal variables in space show to be the gauss nodes of the fem grid. The initial value problems and algebraic equations form a DAE system of index 1. Hereby the discontinuous right hand side of the evolution prevent implicit integration schemes to succeed. The smoothing of these discontinuities allows implicit integration with the drawback of small stepsizes and an increased stiffness in these regions. Another problem especially with the quasistationary approach is, that $\dot{\epsilon}$, that is needed in the heat equation, is not available. Gathering this information without intermixing the model and the numerical discretization is possible by introducing an additional DAE of index 2, that keeps track of ϵ in a separate process. State of the art solution methods use return mapping algorithms combined with low order explicit integration schemes with fixed stepsize. By the interpretation of the problem as PDAE also higher order methods with stepsize control come into scope.

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Data Evaluation as Source For Modelling in Nano-Imaging

B. Alles, Technical University Munich
E. Cotte, Advanced Mask Technology Center Dresden
B. Simeon, Technical University Munich

Corresponding Author: B. Alles
Advanced Mask Technology Center Dresden
Raehnitzer Allee 9, 01139 Dresden, Germany
Phone: +49/(0)351/4048-397
E-Mail: benjamin.alles.external@photomask.com

For more powerful chips manufacturers have to shrink features. As a result functional efficiency is becoming more and more sensitive to placement errors. Due to this issue, the allowed relative positioning error between two consecutive layers — called *overlay* — is tightened heavily. Hence, limits for placement error on masks— called *registration*— are becoming more rigid. These days masks shops are searching for ways to meet required specifications regarding registration, see [1].
Mathematically speaking, registration is a function reg which assigns to every point (x, y) of the mask's front side $\mathcal{M} \in \mathbb{R}^2$ its deviations $(\mathrm{dx}, \mathrm{dy})$:

$$\begin{aligned} \mathrm{reg} : \mathcal{M} \quad &\to \mathbb{R}^2 \\ (x, y) &\to (\mathrm{dx}, \mathrm{dy}) \,. \end{aligned}$$

Since only a finite number of points are measured, a registration data set consists of four vectors: two for the coordinates of the measurements points $\mathbf{x}$, $\mathbf{y}$, and two for their deviations $\mathbf{dx}$, $\mathbf{dy}$.
Starting with this problem, a general method will be proposed for analysing data sets (like registration). Here one needs to distinguish between statistical noise of the measurement (or the production process) and a systematic behaviour. One can only correct for the latter part. A possible correction method will be shown at the end.
While statistical noise is changing arbitrarily in each measurement point, one expects a systematic behaviour to be smooth and vary slower. Using those properties smoothing splines seem to provide a suitable approach for extracting systematic fingerprints. The smoothing spline g is the function that minimizes the follwing expression for $g \in \mathcal{C}^2(\mathbb{R}^2, \mathbb{R})$:

$$\sum_{i=1}^{n} \left(Z_i - g(x_i, y_i)\right)^2 + \lambda \int_{\mathbb{R}^2} \left(\frac{\partial^2 g}{\partial x^2} + \frac{\partial^2 y}{\partial y^2} + 2 \frac{\partial^2 g}{\partial x \partial y} \right)^2 , \tag{1}$$

where $\lambda \geq 0$ is referred to as smoothing parameter and Z_i is the measured value at x_i and y_i. For $\lambda \to 0$ the smoothing splines coincides with the interpolation spline, while for $\lambda \to \infty$ the spline approximates the (linear) regression line. The construction of such a spline is shown in [2].
One can recognize in expression (1) a roughness penalty, since every curvature increases its value.
With a proper value for the smoothing parameter one should be able to extract the systematic part. Since no theoretical description exists for the systematic behaviours identified in this manner, the validity of this data evaluation must be justified by testing the residuals, e.g. with the Dagostino-Pearson-Test, also known as omnibus-test.
By applying smoothing splines a method is derived that allows — without any use of theoretical analysis or modelling — to improve mask registration if data from similar masks is available. Finally, first results of simulations of this correction method are shown.

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Proceedings
5th MATHMOD Vienna

Modelling and Simulation for Control System Design, Coordination and Supervision

Design and evaluation of control algorithms for nitrogen removal in activated sludge plant: a simulation study

A. Stare, N. Hvala, D. Vrečko and S. Strmčnik, JSI, Slovenia

Corresponding Author: A. Stare
Department of systems and control
Jožef Stefan Institute,
Jamova 39, 1000 Ljubljana, Slovenia
Phone: +386 1 47 73 798, Fax: +386 1 42 57 009
email: *aljaz.stare@ijs.si*

Carefully conducted model-based simulation studies can greatly support the evaluation of control strategies for wastewater treatment plants and, eventually, their implementation in practice. Recently, a simulation benchmark of activated sludge process has been developed within the European COST action 628 and 624 for objective control performance evaluation. The benchmark is a simulation protocol defining a plant layout, a process model, influent loads, test procedures and evaluation criteria.

Cost-effective solutions that give desired effluent quality at minimal operational costs have become increasingly important in the control and operation of wastewater treatment plants. One way to reduce operational costs such as pumping energy, aeration energy and dosage of different chemicals is to implement advanced control algorithms. In this paper several control algorithms for nitrogen removal were designed and evaluated in the benchmark. Both, simple pragmatic and more complex control algorithms were sought. Implemented simple control algorithms were: (1) constant oxygen transfer rate and constant external carbon flow rate, (2) constant external carbon flow rate and oxygen PI control, (3) ammonia nitrogen cascade PI control and PI control of nitrate, (4) ammonia nitrogen feedforward – feedback (FF-PI) control and PI control of nitrate. On the other hand complex nonlinear model based predictive controller was also used to find out what can be achieved with such an advanced control algorithm. In this case the whole benchmark model was used as the internal model of the predictive controller, while also all influent disturbances were assumed to be known in advance.

The main objective for each control algorithm was to keep effluent ammonia nitrogen and total nitrogen below the defined effluent limits. Additionally, overall plant costs were calculated and compared to each other. It is shown that a significant reduction of overall costs can be achieved with the introduction of relatively simple PI and FF-PI control algorithms. However, additional improvements are also possible by using advanced model based control algorithms.

MODELLING OF HYDRAULIC ELEMENTS FOR DESIGN AND SUPERVISION OF HYDRAULIC PROCESSES

M. Golob, B. Bratina, B. Tovornik, University of Maribor, FERI, Slovenia

Corresponding Author: M. Golob
University of Maribor, Faculty of Electrical Engineering and Computer Science
Smetanova ulica 17, 2000 Maribor, Slovenia
Phone: +386 2 220 7161, Fax: +386 2 251 1178
email: mgolob@uni-mb.si

In this paper a different modelling approach for modelling of hydraulic systems is presented. The modelling approach deals with how to obtain adequate mathematical models of most common hydraulic elements as are control valves, tanks, pumps and pipelines, which are often used in process industries. Partial models should be suitable for behaviour simulation of the complete hydraulic system, for simulation of hydraulic process control applications, for supervision of hydraulic processes, and for educational purposes. All partial models (model of pump, model of pipeline, model of tank, and model of control valve) are logically and properly connected together in Matlab/Simulink environment and form the mathematical model of desired system. The difference between classical and presented approach is explained where a non-linear and linearized models of all hydraulic elements tanks are derived. The hydraulic process is simulated and results show the potential of the presented modelling approach. In this paper only ideal fluids or "non-compressible" media are considered, meaning that the possibility of mass conservation in the pipelines is neglected and hydraulic shocks in the system are intentionally avoided.

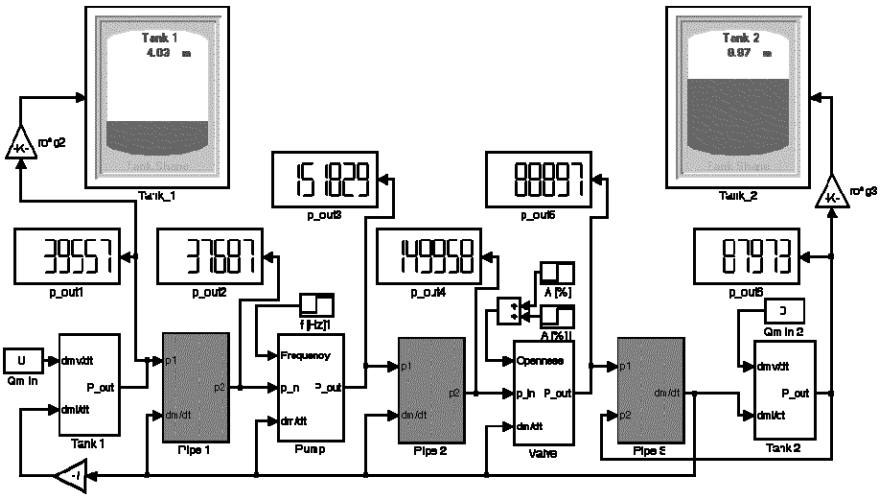

Fig. 1. The two-tank model formed by partial models in Matlab/Simulink (partial pressures [Pa] at time *t=450 s*)

The derivation of partial hydraulic models for modelling of hydraulic systems on the basis of mass and momentum balance equations was presented. By considering the main hydraulic parameters that affect the mass flow along the pipeline or the particular hydraulic element of the system, partial models of the process were obtained (model of pipeline, valve, pump). The obtained partial hydraulic models have to be properly logically connected together so various hydraulic process models can be formed. The behaviour of the two-tank process was simulated and tested in Matlab/Simulink environment, where dynamic properties and the behaviour of the system in comparison to the classic modelling approach is better defined. Still, some limitations of the presented approach exists, for instance the mass flow along the system can be mathematically positive or negative and the model (input and output pressure differences) should be properly adapted, though the partial resistances in the system are always positive regardless to the mass flow direction. Other mechanical characteristics of the materials and system structure should also be considered (viscosity, pipeline angles) in order to improve the mathematical models of the partial elements and therefore the complete model of the process ass well. By modular structure of hydraulic processes one can form various process models and study their behaviour or the behaviour of its' partial elements (the process of pipeline, valve, pump and/or tank). The presented modelling approach is also appropriate for modelling and supervision of big scale water plant systems such as water distribution systems and remote heating systems.

SIMULATION ENVIRONMENT FOR REAL TIME VERIFICATION OF CONTROL ALGORITHM.

ALEXÍK Samuel, ALEXÍK Mikuláš
University of Žilina, Slovak Republic, Department of Technical Cybernetics
samo@frtk.fri.utc.sk, alexik@frtk.fri.utc.sk

Based on present experience, the laboratory verification and teaching of control algorithms in described HLS simulation provide good results. This way, classical and adaptive PID, PIDD^2, DB(n), eDB, eDB-d, algorithms, state algorithms, sliding mode algorithms were verified. This paper described four simulation environments for control algorithms verification. Simulation experiments with digital models of controlled systems and real time HLS simulation were realised in program environment of ADAPTLAB, developed and realised by author. This environment is suitable for developing and verification of classical as well as adaptive control algorithms for SISO and MIMO control loops. The program can be used in three basic modes: described later. The environment also helps developing and verification of new adaptive control algorithms. Up to now experience of author showed, that HLS simulation is more appropriate as digital simulation both for verification and teaching.

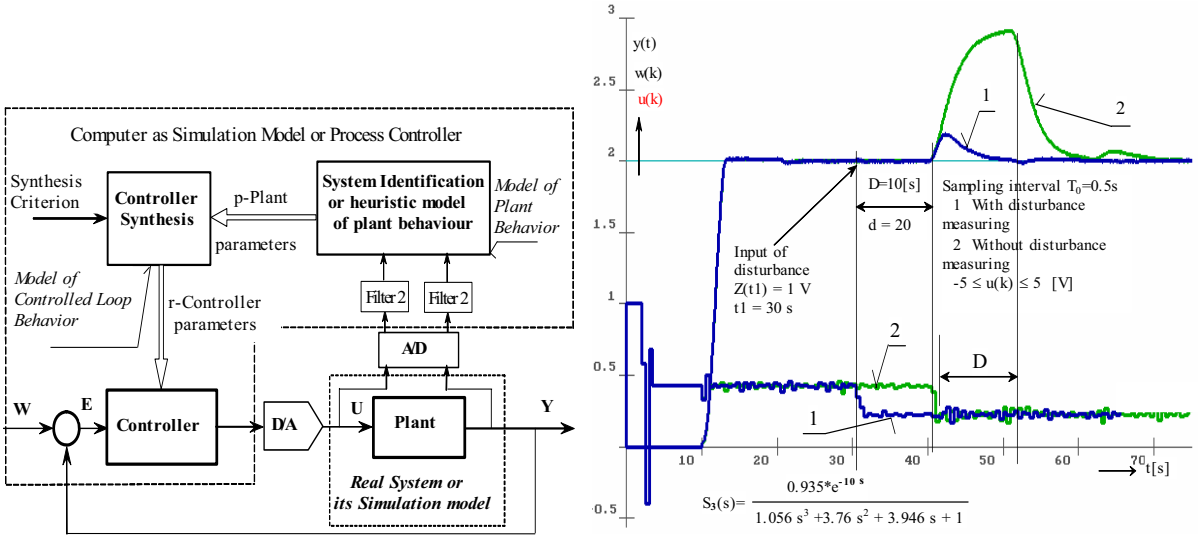

Figure 1 a) b)

a) Adaptive control based on on-line identification b) Hybride simulation- control of the plant with dead time

Transfer function which described controlled plant behavior can be realized by next mode:
a) Analogue model of the processes realized by analogue hardware. This possibility is described in the section3.1. The problem is the realization of time delay, which is needed for some transfer functions .
b) Analogue model of the processes realized by FPAA – Field Programmable Analogue Array. For example FPAA based on Anadigm Designer – AN-220D04.
c) Hybrid model of the processes, realized by any microcontroller + A/D and D/A converters. At present this mode is realised on microcontroller ATMEL K6R4016C1D and ATMEGA8-16PI. In this mode the realization of time delay, varying parameters and nonlinearities is possible.
d) Model of the processes is realized by digital computation of processes' behavior in real time on PC and input to the process / output from the process is realized by A/D or D/A converters. This means that in addition to measurement mode, twice as much converter is needed, because output/input to the controlled plant have to be in analogue mode. In this mode is also possible to realize varying parameters, nonlinearities and time delay.
In all modes, the control algorithm is computed in real time and A/D and D/A converters realize connection to plant.

ACKNOWLEDGEMENTS

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COMPUTER AND PHYSICAL SIMULATIONS COMBINED TO SUPPORT THE DEVELOPMENT OF A NEW AIRCRAFT FUEL MANAGEMENT SYSTEM

J. M. Giron-Sierra, M. Seminario, J.F. Jimenez and C. Insaurralde

Corresponding Autor: J.M. Giron-Sierra
Dep. ACYA, Fac. Fisicas, Universidad Complutense de Madrid
28040 Madrid, Spain
Phone: + 34 91 394 4387, Fax: + 34 91 394 4687
e-mail: gironsi@dacya.ucm.es

A new distributed aircraft fuel management system [1,2] is under development, being the main target of an EU Research Project. The system is based on the use of smart components, such valves, pumps, gauge sensors, etc. The conventional centralized fuel management system architecture, with a central computer and point-to-point connections, is to be substituted by a completely distributed system around a fieldbus [3,4], where the central computer is eliminated.

A fundamental idea of the research is to make the smart components [5] take own decisions on when to act along a system operation. For instance, a refuelling valve decides when to close, based on knowing what is the current system operation and the quantity of fuel in the tanks. Any decision of the smart components is broadcasted to the complete system. For each system operation and each component there exist one local automaton who determines the component reaction when pertinent events happen. The implementation of the ideas to constitute the new distributed system, requires several steps along the research. Firs, the viability of concepts must be shown. Second, software must be developed under constant testing. Third, complete testing of the system operations must be achieved.

Two levels can be distinguished in aircraft fuel systems. Fuel flow, pipes, tanks, pumps, etc. is one of the levels (the fuel handling level). The other is formed by microcontrollers, interface circuits, and the fieldbus (the electronics level).

A combined simulation system has been designed and built, to support the several steps of the research. The paper focuses on this simulation system. It consists of two subsystems. One is a laboratory scale physical simulator of the two levels of the fuel system, using tanks, pumps, microcontrollers, etc. The other is based on two interconnected computers, one of the computers simulates the fuel handling level, and the other simulates the electronics level. Both subsystems can be interconnected, to mix hardware and software simulation.

An advantage of the laboratory scale simulator is that monitoring of messages loading in the fieldbus can be done easily. This is important to know how sure the communications are in such a critical aircraft system. A second advantage is that certain malfunctions or system problems (such a false contact, or a leak) can be introduced and studied. The advantage of computers is that software modifications can be easily introduced, to see the effects.

The paper describes the simulation systems, with special detail in a helicopter case. Some experiments are shown.

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MODELLING AND IDENTIFICATION OF A LABORATORY HELICOPTER

G. Karer and B. Zupančič, University of Ljubljana

Corresponding author: G. Karer
Faculty of Electrical Engineering, University of Ljubljana
Tržaška 25, 1000 Ljubljana, Slovenia
Phone: +386 1 4768701, Fax: +386 1 4264631
email: gorazd.karer@fe.uni-lj.si

In the paper, modelling and identification of a laboratory helicopter with the final aim to design a control system is presented. Modelling and simulation are very important approaches for designing control systems. Therefore, laboratory set-ups, which model real processes, and mathematical models have a significant role. The CE150 is a laboratory helicopter made by Humusoft. It is used for studying system dynamics and control engineering principles from the theoretical point of view and enables a wide range of practical experiments in the fields of modelling, simulation and control. The goal of modelling and identification is to prepare a basis for the students' laboratory assignments, such as designing a multivariable controller that ensures satisfactory control in the whole operating range.

The laboratory helicopter set-up (see figure 1) comprises a helicopter body carrying two motors, which drive the main and the tail propeller of the helicopter, and a servomechanism, which shifts the centre of gravity by moving a weight along the helicopter's horizontal axis. The helicopter body is connected to a base so that two degrees of freedom are enabled, i.e. rotation around the horizontal axis nad rotation around the vertical axis. However, it is possible to fix one (or both) degree of freedom by tightening the intended screw(s) in the helicopter base when needed. The axes of the main and tail rotor and the vertical and horizontal helicopter axis are perpendicular to each-other. The helicopter model can be represented as a non-linear multi-variable system with two inputs (u_1 and u_2) and two outputs (y_ψ and y_φ).

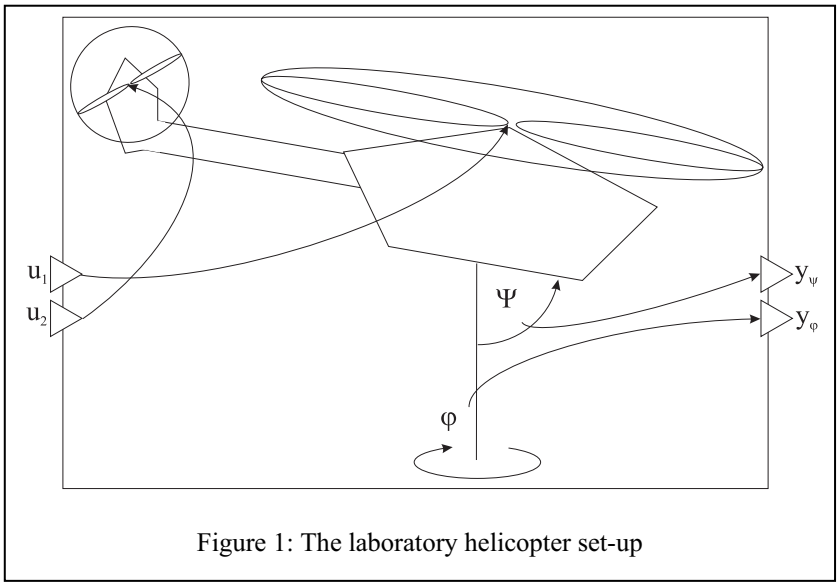

Figure 1: The laboratory helicopter set-up

There are two well known modelling approaches: theoretical and experimental. Usually, both approaches have to be combined, which is also the case in modelling of the laboratory helicopter. In the paper, theoretical and empyric modelling is systematically described. Identification of the necessary parameters is tackled and the results are presented. Finally, model validation is discussed and a simple control approach is proposed.

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MODELLING AND SIMULATION IN DEVELOPMENT AND TUNING OF INTELLIGENT CONTROLLERS

E. K. Juuso, University of Oulu, Finland

Control Engineering Laboratory
P.O. Box 4300, FIN-90014 University of Oulu, Finland
Phone: +358 8 553 2463, Fax: +358 8 553 2304
email: esko.juuso@oulu.fi

In industrial applications, operating conditions are often changing so strongly that the changes in nonlinearities must be taken into account. The adaptation mechanism can be either on-line or predefined. Linguistic equation (LE) controllers can combine various control strategies [1]. The new methodology was tested in a solar collector field where a trial and error type controller tuning does not work since the operating conditions cannot be reproduced or planned in detail because of changing weather conditions [2]. All the parameters of the multilevel controller are tuned with a training set which contains a balanced selection of control tasks. There are totally 34 parameters for nonlinear scaling and weighting the actions.

Genetic algorithms based on binary coding of the parameters provide a good overall operation of the control system. Model-based predictive control (MPC) is a good solution for start-up and load disturbances in a solar power plant, and it works well for smoothly changing operating conditions. However, normal MPC has difficulties in coping with quickly changing operating conditions, e.g. cloudy conditions or load disturbances in solar power plants. A braking action based on analysing the speed of the change was the first solution: following a good trajectory is built in. The braking action is implemented by a correction factor that increases the importance of the change of error when the temperature goes towards the set point. As the performance will change too much before the feedback controller detects the difference, some additional feedforward control actions are taken in a properly scheduled way, i.e. the additional control actions become first gradually stronger and then slowly disappear.

Both the braking action and the feedforward compensation of the load disturbance have been tuned with combined dynamic simulation and MPC. Dynamic simulation with LE models is a very fast and reliable method for comparing alternatives. For the control design, a realistic dynamic behaviour, including oscillations, is necessary, and this was achieved in these models. After tuning the new LE controller has the same performance as the MPC in smoothly changing operating conditions, but in addition to this the new controller can cope with multiple disturbances, e.g. load disturbances in cloudy conditions. The new adaptive technique has reduced considerably temperature differences between collector loops.

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OPTIMAL MULTIVARIABLE CONTROL DESIGN USING GENETIC ALGORITHMS

M. Atanasijević-Kunc, A. Belič, R.Karba
Faculty for Electrical Engineering, Ljubljana, Slovenia

Corresponding Author: M. Atanasijević-Kunc
Faculty for Electrical Engineering
Tržaška 25, 1000 Ljubljana, Slovenia
Phone: ++386 (0)1 4768-314, Fax: ++386 (0)1 4264-631
email: maja.atanasijevic@fe.uni-lj.si

Abstract

For the separation of mixed components on the basis of volatility, different kinds of distillation are used in chemical industry. In the paper the binary semibatch-rectification process is presented. Nonlinear model is first used for the evaluation of different operating strategies. Analysis results have indicated that for higher concentrations (80%) of the final product and increased mass of the product suitable control action is needed.

For this purpose multivariable controllers were designed in several steps and compared regarding their complexity and quality of process operation.

The first presented result is a robust MIMO-P controller while the other two are time - varying MIMO nonlinear controllers with P and PID - structure and were tuned using GA - optimizaton. The design flow was oriented in such manner that the information from previous design steps was taken into account in the next one which has shortened the optimization procedure.

The efficacy of design results is illustrated in Figs. 1 and 2, where the mass and the concentration of the final product are compared for three solutions.

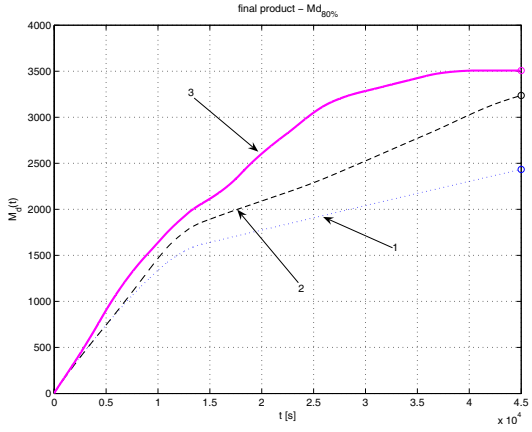


Figure 1: Mass of the product

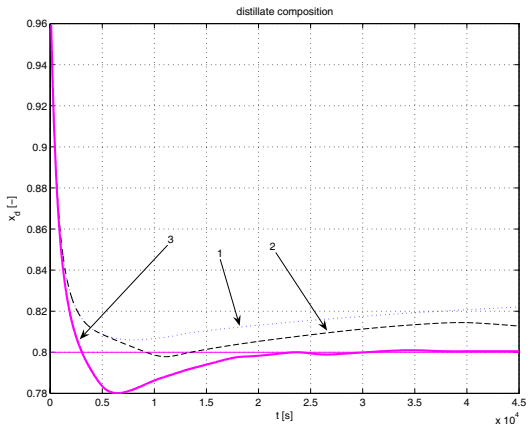


Figure 2: Concentration of the product

The first solution increased the mass of the product almost seven times regarding the situation, where the system was guided by the operator. Time varying controllers can further improve the quantity of the product regarding the first solution for 33% and 44%, while in the last case the batch can finish approximately two hours earlier.

COMPARISON OF LEARNING ALGORITHM BASED ON SLIDING MODE AND NEURAL NETS CONTROL BY REAL TIME SIMULATION

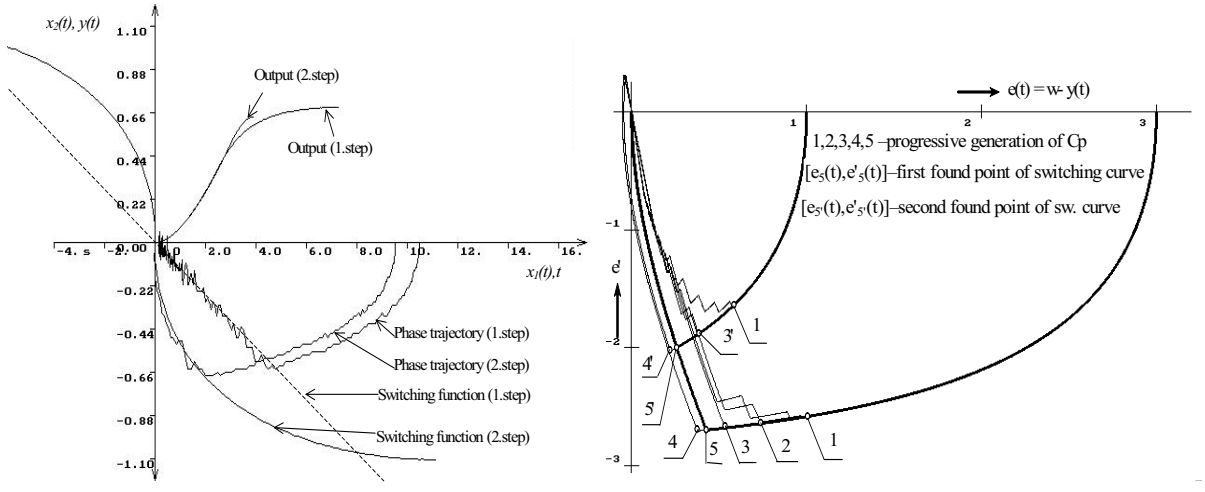
ALEXÍK Mikuláš, LUČIVJANSKÝ Marek

University of Žilina, Department of Technical Cybernetics, Slovak Republic
E-Mail: alexik@frtk.fri.utc.sk, lucivjan1@post.sk

In many practical applications especially in servomechanism, the t-optimal control problem is usually solved for desired system and then applied with the specific control rules. For class of second order systems with single input and single output sliding mode control is used. If the system is not stationary or there is a possibility of the system parameters change, the classical sliding mode control couldn't be used and the learning controller based on sliding mode control could assign the optimal control requirement. The paper describes two learning algorithms. The first is based on classical sliding mode control and the second on sliding mode control combined with the neural networks. The first algorithm is clearer, but learns slowly. The second algorithm which uses neural networks learns more quickly and to understand it fully it is crucial to know how the first one works. Both learning algorithms described in the paper set the t-optimal switching surface for second order controlled system. The combined algorithm can do so even for third order controlled system.

Fig. 1 The laboratory carriage model

The parameters change means that carriage-load changes. There are five various carriage-loads and therefore a system with five different parameter couples. The only a priori condition is the existence of the initial stabile control, for example the sliding mode control based on switching curve and switching line. Described algorithm was tested on laboratory equipment by real time simulation experiment



a) b)

Fig. 1 Time suboptimal learning control based on a) neural nets+ sliding mode b) sliding mode

ACKNOWLEDGEMENTS

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SIMULATION ENVIRONMENT FOR THE INVESTIGATION OF AUTOMATIZED COOPERATION OF MARINE CRAFTS

D. M. Carrillo, J.A. Lopez-Orozco, J. M. Giron-Sierra

Corresponding Autor: J.M. Giron-Sierra
Dep. ACYA, Fac. Fisicas, Universidad Complutense de Madrid
28040 Madrid, Spain
Phone: + 34 91 394 4387, Fax: + 34 91 394 4687
e-mail: gironsi@dacya.ucm.es

There are marine operations, such spill over confinement, towing, rescue, etc., which involve the cooperation of several ships. In particular, the recent sinking of the "Prestige" oil tanker near the Spanish coast has shown some issues requiring further analysis. For instance, it was noticed that the usual operation for oil spill over confinement consists in two ships towing a boom. Running some simulations in the environment described in this paper, put into light several coordination difficulties arising with just two ships towing the boom. More than two ships for this task cause still more difficulties. In such a case, the help of automatized real-time coordination procedures would be useful. This can be made with computers on board the ships, bringing advice to the ship captains. The purpose of our research is to add automatization to marine operations. The on-board computer interacts with the ship captain in a verbal form. All computers communicate and think about the operation evolution, to help captains to take optimal decisions for a good achievement of the general operation.

An important step for the research is to establish a simulation environment for the analysis of operations with several cooperating ships. The paper describes a first version of the environment. Some experiments about formations of ships have been already done, offering an interesting basis to analyse cooperation difficulties and possible solutions. As reflected by the scientific literature, the research on ships working together has started recently. Several different scenarios have been considered. For instance [1] about towing, or [2] about ship formation control. The general approach is to extend to the marine context a main stream of contemporary research about multirobot systems [3,4].

The main approach of the simulation environment: is that each ship is an agent. Each agent obeys to behaviour rules that are specified using the simulation facilities. The simulation environment is made with MATLAB-SIMULINK. Two simulation experiments about formation control are described, highlighting interesting phenomena. Figure 1 shows the trajectories of 5 ships, starting from a random initial position and evolving to attain a formation with all ships in parallel. The coordination strategy in the example is "follow-the-leader". Ships have sway motions when they turn. Figure 2 shows the trajectories when the ships evolve to attain a single line formation. An analysis of the individual motions show the same effects noticed by car drivers in slow traffic.

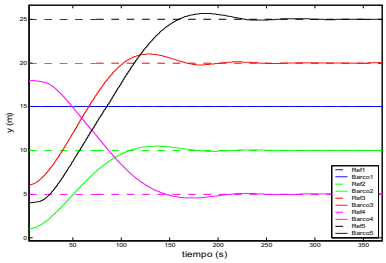

Figure 1: Formation of ships in parallel.

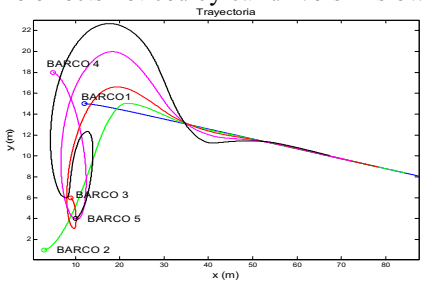

Figure 2: Single line ship formation

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MODULAR SOFTWARE ENVIRONMENT FOR GENERAL PURPOSE AUTONOMOUS AGENTS SIMULATION AND CONTROL

S. Cifuentes, J. M. Girón-Sierra, J.F. Jiménez

Corresponding Author: J. M. Girón-Sierra
Facultad de Físicas
Dto. Arquitectura de Computadores y Automática
Universidad Complutense de Madrid
Phone: +34-91-394-4389; fax: +34-91-394-4687
e-mail: gironsi@ dacya.ucm.es

Cooperative behaviour has rise in recent time a huge interest in the scientific community. There are many different disciplines interested in the issue: Animal Ethology, trying to explain natural grouping behaviour like herbs, flocks, warms and schools, Automatic Control trying to mimic the apparently simple and highly decentralised control strategies observed in natural grouping behaviour, Robotics trying to develop elementary animal-like robots that will be able to perform together no so-elementary tasks, Artificial Intelligence trying to model the reasoning methods to generate emerging behaviour, etc.
A recent workshop held in New York [1] focused its interest not in the goals achieved until that time, "but rather to delineate common ground and to identify fundamental unresolved problems".
The list of unresolved problems in which, currently, there is active research is too wide as to be summarized in a few lines. It is possible to stand out, among others: vehicle formation (in particular for non-holonomic vehicles) [2], Gathering of autonomous robots [3], Cooperative Surveillance [4], Common Search [5] and Cooperative Rescue [6]. These so called cooperative scenarios lead to other more fundamental problems: communications, sensors fusion, leadership, robustness against failures, awareness, etc.
Focussing in the specific field of robotics, there has been several attempts to establish some king of taxonomy for system composed by multiple robotic agents [7]. These Classifications are usually based on robots cooperation and coordination capabilities, which are considered as crucial features of the resulting team.
Virtual and actual autonomous agents share some common properties but also present significant differences, being perhaps the most remarkable the uncertainty and incompleteness on information acquired from environment [7] in the actual case. This lead to the apparent paradox that no actual multiagent system should be built up before its design has been soundly probed and no design can be soundly probed before being actually built.
As in many other knowledge areas, it is possible to develop software simulator that permits to resemble, at least partially, the behaviour of the agents.
The present work describes a general purpose software environment specially designed for this task. Agents and scenarios can be prototyped in a modular way and so, departing from very simple agent models, it is possible to increase gradually is complexity until reach more elaborate behaviours. Additionally, this software tool takes full advantage of each model which once developed can be reuse in many different scenarios or be furnished with new features added to the original ones. At last but not the least, it is possible to connect the program to actual robotic agent (employing a radio link) to monitor their behaviour or to control them.

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Rule Based Automation of Engineering in Process Industries

ON RULE BASED AUTOMATION OF AUTOMATION

STEFAN SCHMITZ, ULRICH EPPLE
Corresponding Author: Stefan Schmitz
Chair of Process Control Engineering - RWTH Aachen University
Turmstraße 46 - D-52064 Aachen, Germany
Phone: +49 (0) 241 80 97613
Fax: +49 (0) 241 80 92238
EMail: Stefan.Schmitz@plt.rwth-aachen.de

Installation of new plants, machines, and functionality is always associated with high expenses. A considerable part of these expenses is owed to the engineering of process control engineering functions. Currently this work can only be done manually. A proper way of decreasing expenses is to automate the engineering process.

The development of autonomous functions, respectively tools that are able to manipulate the existing process control system or the process control itself, is called Automation of Automation (AoA or AdA[1]). Usually this development refers to the automated basic automation of process control functions or interlock recognition and implementation (cf. [2, 3, 4]). Diagnostic functionality is also a current topic (cf. [1]).

The majority of existing solutions uses a specific tool and needs a (special) interface to the process control system. Special tools are always synonymous with proprietary solutions, with all known pros and cons. Instead of a new specific solution a general concept of completely integrated rule based control functions respectively Automation of Automation functions is introduced. This concept claims the existence of a general rule representation in the form of "if A then B". This rule is mapped to continuous function charts inside the process control system. Test (if A) and Production (then B) are represented by a new set of function blocks.

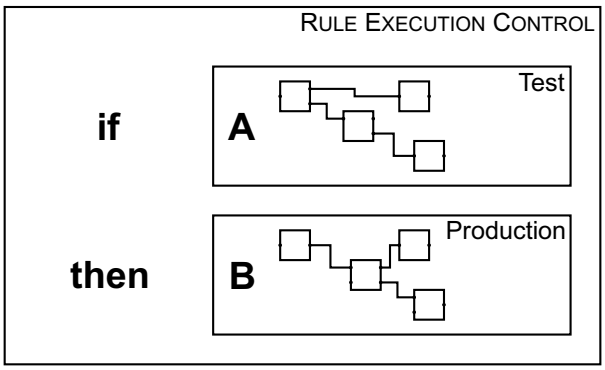

Figure 1: Basic Principle of a completely integrated Automation of Automation

The concept not only allows the basic automation engineering but also a multiplicity of other Automation of Automation applications like documentation, alarm management and so on. The ability to manipulate the instance network of the process control system online creates further areas of application outside the scope of automated engineering.

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RULE BASED ENGINEERING OF ASSET MANAGEMENT SYSTEM FUNCTIONALITY

T. Schmidberger, Helmut-Schmidt-University, till.schmidberger@hsu-hh.de
A. Horch, ABB Corporate Research Ladenburg, alexander.horch@de.abb.com
A. Fay, Helmut-Schmidt-University, alexander.fay@hsu-hh.de
R. Drath, ABB Corporate Research Ladenburg, rainer.drath@de.abb.com

Corresponding Author: T. Schmidberger
Helmut-Schmidt-University/ University of the Federal Armed Forces Hamburg
Holstenhofweg 85, 22043 Hamburg, Germany
Phone: +49 (0)40 6541-2741, Fax: +49 (0)40 6541-2004
email: till.schmidberger@hsu-hh.de

Technical realisation and costs are the two main contrary aspects meeting during the whole lifetime of a plant. Both aspects should be taken into consideration if the efficiency, productivity and safety of plants are discussed. The aim of the total plant engineering is to find the balance between the total lifetime costs, plant performance and risk [1]. So-called Asset Management Systems (AMS) are introduced to support these tasks. AMS include all actions to save the reliability and the value of a plant [4]. It is the task of an AMS to establish a balance between asset performance and the investment / maintaining costs of asset management functionality. The performance and efficiency of an AMS can be measured in terms of cost and downtime avoidance.
The Plant Asset Management (PAM) is a sub-domain of Asset Management (AM) and focuses on the avoidance of unintentional downtimes caused by technical failures. It is the task of the plant process control engineering to establish asset management functionality for a given plant with a given process. “Online Plant Asset Management includes assessment of the plant, decisions on maintenance measures and their execution.” [4] PAM should support the operators to keep the production running. This covers maintenance, equipment assessment, repairs and substitution of equipment. The importance of PAM can be clarified by the simple fact that a rather inexpensive field equipment item can cause cost intensive downtimes and damages.
On the other hand, the AM functionality has to be added to the system, which requires significant engineering effort and causes further engineering costs. Due to these engineering costs, plant owners/operators hesitate to make use of the AM systems’ functionality.
This paper describes a method to automate parts of the engineering of an AM, thus reducing the engineering costs and making AM systems more attractive. We focus on the AM functions which are based on the evaluation of several process values, check them for consistency, and thus detect erroneous/illogical value combinations indicating either a defect of a sensor or actuator or a defect of a plant component related to them. These AM functions can be implemented e.g. in a PCS, which already has access to all the required process variables. The paper describes a method which allows to automate the engineering process for asset management functionalities, if combined with an object / aspect oriented data model, which stores the plant engineering information [3]. Software programs are able to access the electronically stored plant data and can use the information and interpret them. The introduction of a rule based engineering approach allows an analytical evaluation. It uses the electronically stored plant information to identify component assemblies. Their process values are a part of an AM function. The instantiation of a resulting AM function into the PCS is performed automatically.

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A RULE ONTOLOGY AS A BASIS FOR AUTOMATIC REASONING ON INDUSTRIAL PLANT INFORMATION

T. Schmidberger, Helmut-Schmidt-University, till.schmidberger@hsu-hh.de
R. Drath, ABB Corporate Research Ladenburg, rainer.drath@de.abb.com
A. Fay, Helmut-Schmidt-University, alexander.fay@hsu-hh.de

Corresponding Author: T. Schmidberger
Helmut-Schmidt-University/ University of the Federal Armed Forces Hamburg
Holstenhofweg 85, 22043 Hamburg, Germany
Phone: +49 (0)40 6541-2741, Fax: +49 (0)40 6541-2004
email: till.schmidberger@hsu-hh.de

Neutral, tool-independent file formats, like CAEX [5], store industrial plant information in hierarchical object models. Some of them are standardized. They are used as data exchange formats between CAE-tools for plant design and process control engineering tools. Furthermore, they can be seen as the fact-basis for knowledge based systems, which allow the automation of repetitive process control engineering tasks. A prerequisite to analyze the fact basis is the knowledge about the relationships between the facts. This knowledge can be formalized in rules. Today there is no standard rule format for industrial plant information reasoning.
Defining an ontology is like defining a set of data and their syntactical structure. Important terms are the scope, domain and syntax of the ontology [2]. The definition of the scope identifies the purpose of the new ontology [1]. In this case, one has to define the rules which are able to deduce information from the topological plant information. The ontology has to include a set of data and its structure in such a form that computer applications can use them for evaluation. The new rule ontology has to contain the domain specific problem solving knowledge for all control engineering tasks like interlockings and asset management functionalities. The base set of the new rule elements has to be adequate for simple coding of all possible formulas and expressions.
Considering the domain aspect, the new rule ontology should make the automated interpretation of domain knowledge possible. It separates the domain from the reasoning knowledge. The new domain includes rule elements, which are essential for the automatic reasoning process. The rules describe events being raised because of a special cause. Such action-reaction behaviour has to be supported by the ontology. It can be literally expressed with the "if … then …" formulation.
Instead of developing a completely new ontology, existing ontologies have been evaluated, in particular RuleML [4] and MathML [3], and have been re-used for the rule ontology: MathML has been chosen as basis for the description of all mathematical aspects. It is supplemented by some "string-handling" elements. Some of these new element names are derived from their usage in programming languages. Additional rule information, like references to the CAEX data, is encoded in the CAEX style.
A software program has been designed and implemented to prove the suitability and practicability of the automatic reasoning with the developed rule ontology. The software application allows the evaluation of the plant data and the instantiation of asset management functionalities. The work described in this paper can be seen as the first step towards a standard rule ontology for process industry reasoning tasks.

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Automated Treatment of Balances

Reiner Jorewitz, Ansgar Münnemann, Ulrich Epple
Chair of Process Control Engineering – RWTH Aachen University
Rüdiger Böckler, Wolfgang Wille, Ralf Schmitz
INEOS

Corresponding Author: R. Jorewitz
Chair of Process Control Engineering – RWTH Aachen University
Turmstr. 46, 52064 Aachen, Germany
Phone: +49 (0)2 41 80 – 9 77 33,
FAX: +49 (0)2 41 80 – 9 22 38
EMAIL: jorewitz@plt.rwth-aachen.de

In order to improve the plant performance, advanced functions have to be included in addition to the basic automation. Most of those functions fulfill analysis duties, e.g. control loop optimization, asset management and performance monitoring. Because of the increased engineering effort the automation of engineering – called "Automation of Automation" – has to be applied. Last but not least, due to the dominance of the object-oriented paradigm, this means in almost all cases rule-based object manipulation.
For the automation of performance monitoring in the process industry, the RIVA model ([1]) has been developed. One central part of this approach is the treatment of balances, for data reconciliation as well as for the enrichment of the plant data model. Since the handling of balances plays such an important role and is applicable to other fields, e.g. logistics, this paper focuses on data models, rules and algorithms concerning balances.

A generic representation for dealing with balances contains the following elements

- a model for the measurable and the balanceable quantities and their relations,
- material laws describing the functional dependencies of the balanceable quantities on the measurable quantities,
- a model for general basic subsystems, which represent the real world problem started from, and how they interact
- and algorithms performing the handling of the balances.

This paper states principle demands on these elements and gives a possible solution. The first three elements form object networks which are subjected to rules. The model formulation allows or prohibits the automation of certain engineering steps. The algorithms are described by their requirements, not in the notation of a specific rule execution system. It is discussed in detail which balanceable quantities are calculable and which balances can be drawn under various conditions.

By formulating the suggested solution as generic as possible, e.g. making use of meta modeling ([2]), the approach is applicable for various fields of interest. As an exemplary case the chemical engineering field is given.

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Port-based Modelling and Control

THE PORT-HAMILTONIAN SYSTEMS APPROACH TO MODELLING AND CONTROL OF COMPLEX DYNAMICAL SYSTEMS.

WHY SHOULD YOU EVER BE INTERESTED?

Herman Bruyninckx, K.U.Leuven, Belgium

Department of Mechanical Engineering
Katholieke Universiteit Leuven
Celestijnenlaan 300B, BE-3001 Leuven, Belgium
http://people.mech.kuleuven.be/~bruyninc

This presentation gives a "bird's eye" view on the *paradigm* of Port-Hamiltonian Systems (PHS) modelling and control. PHS is a paradigm, in the sense that it provides a set of models, thought patterns, techniques, practices, beliefs, systematic procedures, terminology, notations, symbols, implicit assumptions and contexts, values, performance criteria, ..., shared by a community of scientists, engineers and users in their modelling, analysis, design and application of complex dynamical systems. The name "Port-Hamiltonian" systems refers to the two major components of the paradigm: (i) its modelling is *port-based*, more in particular it builds upon the successful multi-domain Bond Graph way of composing complex systems by means of *energy*-preserving interconnections; and (ii) its mathematical framework is built on the Hamiltonian function, which also considers *energy* to be the basic physical concept for modelling systems as interconnected components. In addition, the PHS paradigm extensively relies on differential geometric formulations, because this is a very appropriate mathematical formalism whenever one wants to separate generic and invariant descriptions from the details and particularities of applications or application domains.

The last few years, significant progress has been made in the PHS paradigm, to a large extent thanks to the concerted efforts of the GEOPLEX project (Geometric Network Modeling and Control of Complex Physical Systems, www.geoplex.cc). Some of the major evolutions are: the PHS approach has excellent results in the systematic separation (conceptual as well as in the mathematical representation) of the *interconnection structure* and the *dynamical properties of interconnected system*; finite-dimensional systems and infinite-dimensional systems can be described with unified concepts and mathematical representations, and one is nearing the breakthrough towards unified *control* of both domains; the *damping injection* and *energy shaping* control approaches (that fit naturally within the PHS paradigm) begin to mature and show their advantages for the construction of safe and predictable controllers for very complex systems.

This presentation outlines and discusses the *systematic procedure* for the modelling and control of complex dynamical systems, as it is beginning to materialise in the PHS community. It will also illustrate how far the PHS approach has already penetrated various seemingly different engineering domains, such as robotics, electrical networks and drive systems, chemical engineering, and mechatronics.

PORT-BASED MODELING OF DYNAMIC SYSTEMS IN TERMS OF BOND GRAPHS

Peter C. Breedveld

Control Engineering Laboratory, Faculty of Electrical Engineering, Mathematics and Computer Science, University of Twente, P.O. Box 217, 7500 AE Enschede, Netherlands
tel.: +31 53 489 2792, fax: +31 53 489 2223, e-mail: P.C.Breedveld@ewi.utwente.nl

Port-based modeling of dynamic systems is the topic of the first chapter of the book that will be one of the main results of the European project 'Geometric Network Modeling and Control of Complex Physical Systems' (GEOPLEX, IST-2001-34166, Key Action, Action line KAIV: Essential Technologies and Infrastructures, Action Line IV.4.2.1). In this chapter the reader is introduced to the concepts needed for port-based modeling, design and reasoning in order to prepare and motivate for the geometrical formulations of the port-based approach in the remainder of the book. After some general remarks about the modeling process, this is done from a historic perspective, which immediately relates the port concept to its original notation, the bond graph. Bond graph notation is discussed as well as the concept of causality, which allows one to combine physical and computational structure into one notation and provides important feedback on modeling decisions in the trade-off between conceptual and computational complexity. Several simple examples of its use are presented and the details of many bond graph related transformations and analysis techniques are discussed in a series of appendices: conversion of an IPM into a bond graph, conversion of causal bond graphs into block diagrams, generation of a set of mixed algebraic and differential equations, direct linear analysis, impedance analysis using bond graphs, nonlinear mechanical systems (mechanisms), homogeneous functions and Euler's theorem, homogeneous energy functions, Legendre transformations, co-energy functions, relations for co-energy functions, Legendre transforms in simple thermodynamics, Legendre transforms and causality, Maxwell reciprocity of constitutive relations.
As it is impossible to fit all this material in this short contribution, two examples of the content are given that are more or less self-supporting/independent, viz. the Glossary, which provides a kind of bird's eye view of the material, and the first Appendix that discusses basic model transformations. However, first the most important basis for the work on port-Hamiltonian systems, viz. the generalization of the bond graph representation into generalized bond graphs, is discussed shortly first.

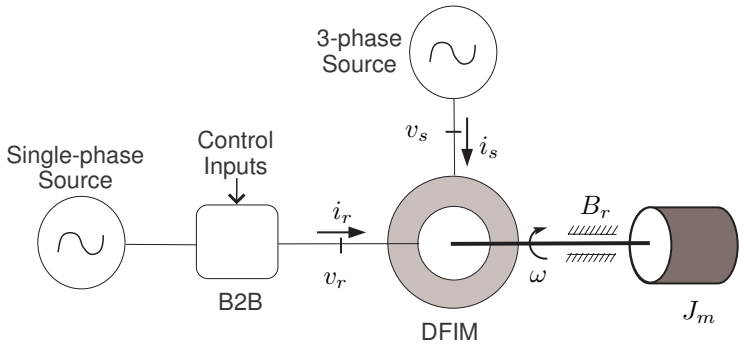
ENERGY-BASED MODELLING AND CONTROL OF A MULTI-DOMAIN ENERGY STORAGE AND MANAGEMENT SYSTEM

Carles Batlle, Arnau Dòria, Enric Fossas, Technical University of Catalonia, Spain,
and Romeo Ortega, SUPELEC, France

Corresponding Author: Carles Batlle
IOC and Department of Applied Mathematics IV
Technical University of Catalonia
EPSEVG, Av. V. Balaguer s/n
Vilanova i la Geltrú, 08800 Spain
carles.batlle@upc.edu

We give an overview of part of the chapter of the Geoplex book devoted to examples, specifically the one which deals with electromechanical systems. We study a rather complex example of a port Hamiltonian system made of two subsystems, presenting each some remarkable characteristics, namely interconnection structures which depend either on the system state or on a discontinuous control variable. The first subsystem, a doubly-fed induction machine (DFIM), like most rotating electric machinery, has a complicated, geometry depending energy function, encoding in a lumped parameter description the interaction of the stator and rotor magnetic fields. After a coordinate change, this dependence can be absorbed into the interconnection structure, resulting in a model which has the additional feature of yielding itself quite easily to the formulation of sensible control problems. The second subsystem, a back-to-back (B2B) power converter made of a rectifier and an inverter, also has, this time from the beginning, an interconnection structure which varies with the topology of the system, and which can be controlled by the state of a set of switches.

The following figure shows the DFIM+B2B interconnection, together with some ancillary elements. This arrangement allows to store and transfer energy to a local load connected to the stator of the DFIM, in parallel with the main power grid.



We describe the detailed port Hamiltonian structure of both subsystems, their interconnection and the design of suitable IDA-PBC controllers for both of them. The associated bond-graph description is also presented, and simulations using `20sim` are run.

A PORT BASED FORMULATION OF TRANSPORT PHENOMENA

A. Baaiu, F. Couenne, D. Eberard, C. Jallut,
L. Lefèvre, Y. Legorrec, B. Maschke and M. Tayakout-Fayolle,
LAGEP, UMR 5007 CNRS/Université Claude Bernard

Corresponding author : L. Lefèvre,
CPE-Lyon Bat 308G, 43 Bd du 11 novembre 1918, F-69622 Villeurbanne Cedex, France.
Phone : +33 4 7575-9464, Fax : +33 4 7543-5642, Email : Laurent.Lefevre@inpg.fr

The goal of this paper is to present an extension of the port-based modelling approach to systems of heat and mass transport. The approach will be illustrated on the example of an isothermal model of the mass transfer phenomena in adsorption processes. This example provides the opportunity to develop interesting extension of the Bond Graph modelling language to (spatial) multi-scale modelling.

Firstly, we present a way to split the classical partial differential balance equations obtained for transport phenomena. Starting from the power continuity equation, we define conjugate power variables as differential forms and the instantaneous power conservation as a generalized interconnection element called Dirac structure [1]. This interconnection structure defines the conservation law which has to be completed by closure equations. The latter are defined as "atomic" subparts of the model whose constitutive equations are classical thermodynamics laws.

Secondly, the assumptions used for the development of the multi-scale model are briefly recalled. The defined multi-scale space of efforts and flows (differential forms) has a natural fiber bundle structure which is outlined. It is shown how the chemical potential continuity and the molar fluxes continuity equations may be used to define again a Dirac structure on this fiber bundle. Finally, the models of the different scales are assembled in a generalized interconnection structure connecting conservative and dissipative elements at the different scales.

The developed model is stated independently from the geometric specifications of the system. This geometry may be defined at the end of the physical modelling process as the derived equations and the interconnection structures are "geometry-independent". These specifications are the object of a companion paper in the conference [2]. The model is a network model where each element represents a specific phenomenon which may be identified from a thermodynamics point of view. The instantaneous power conservation and the description of the power transfers within the system and through its boundaries are explicitly represented with the help of the Dirac structure.

These properties have several important consequences. Firstly, the derived model requires few parameters and these parameters have a clear physical meaning. Secondly, the model is acausal, hence it postpones the choice of boundary conditions and is thus clearly reusable. Finally, the central geometric Dirac structure is a direct generalization of Poisson structure in Hamiltonian systems. It suggests and allows the use passivity-based or energy-shaping techniques for control purposes. These considerations strongly encourage the development of a discretization method which preserves both the nature of the interconnection structures and the physical properties of the connected elements. Simulation results obtained with the help of such a numerical scheme are presented in [2].

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Control of Port Hamiltonian Systems by Interconnection and Energy Shaping via Generation of Casimir Functions. An Overview

A. Macchelli, University of Bologna, Italy
R. Pasumarthy, University of Twente, The Netherlands
A. J. van der Schaft, University of Groningen, The Netherlands

Corresponding Author: A. Macchelli
University of Bologna - CASY-DEIS
viale Risorgimento 2, 40136 Bologna, Italy
Phone: +39 051 2093034, Fax: +39 051 2093073
email: amacchelli@deis.unibo.it

Abstract. In this paper, an overview on the control by interconnection and energy shaping via Casimir generation for port Hamiltonian systems is presented. This control methodology has its origins in the Energy-Casimir method according to which stability can be proved by using in Lyapunov analysis next to system Hamiltonian other conserved quantities. In the control by interconnection, the controller structure is chosen in order to properly introduce such conserved quantities (Casimir functions) and shape the energy of the system such that a minimum in the desired equilibrium configuration can be introduced. In this paper, the basic results on the stabilization of finite dimensional system are summarized and then generalized in order to cope with distributed parameter plant. The stabilization of a set of port Hamiltonian systems interconnected by (dissipative) transmission lines is presented in order to illustrate the design methodology.

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SIMPLE ELASTIC SYSTEMS, AN INTRODUCTION BASED ON GEOMETRY

K. Schlacher, M. Schöberl, H. Ennsbrunner,
Johannes Kepler University Linz, Austria

Corresponding Author: K. Schlacher
Institute of Automatic Control and Control Systems Technology
Altenbergerstraße 69, 4040 Linz, Austria
Phone: +43 732 2468 - 9731, Fax: + 43 732 2468 - 9734

email: kurt.schlacher@jku.at

Simple elastic structures like strings, beams or membranes and plates are basic elements for many engineering fields. But one is often not aware that their mathematical models are approximations of certain equations of linearized elasticity. Mathematical modeling of dynamic systems with methods of classical physics requires two sets of equations. The balance and/or conservation equations express that certain physical quantities or their sum are preserved. In general these equations do not depend on the special behavior of the materials. Conservation of mass or balance of momentum are representatives of this class. The constitutive relations describe the behavior of the materials, typical representatives are Hook's law or friction relations. Within this setting one assumes that balance equations are never violated, whereas constitutive relations are often approximately known only.
Mathematical models of elastic bodies are based on the conservation of mass and the balance of linear momentum and momentum of momentum, see [2, 5, 6]. To simplify this complicated set of partial differential equations, one makes the strong constitutive assumption of the symmetry of the stress. This relation guarantees that balance of momentum of momentum is fulfilled, and we have to take conservation of mass and balance of linear momentum into account only. Additionally in simple elasticity, one assumes the existence of the stored energy function to express certain constitutive relations. If this function exists and the symmetry of stress is met, then the derived mathematical models have the structure of a Lagrangian or Hamiltonian system for a certain choice of the coordinates. Depending on the application one may linearize the balance and/or the constitutive relations. In general one needs three spatial variables and the time to describe the motion of an elastic body. The model of structures, like beams or plates with a small extension in one direction compared to the others, can be approximated by reduced models with less spatial variables. This way, the models of beams, plates, etc. are derived by the reduction of the linearized equations of simple elasticity. Of course, if the reduction process preserves the Hamiltonian or Lagrangian structure, then the resulting models will have this structure, too.
After a short introduction into basic elasticity we present the equations of motion for simple elastic systems. We confine ourselves to the time invariant case and assume that physics takes always place in an inertial space with Euclidean coordinates, for the general case see e.g. [4]. A fundamental property of the derived equations is that one can rewrite them in the Lagrangian or Hamiltonian form, see [1, 3]. Often, the original equations are too complex, and one tries to construct simpler models. This can be achieved by adding additional constraints. How one obtains the reduced model based on the Lagrangian or Hamiltonian description or directely from the equations, will be discussed in general and demonstrated with the help of two examples, the rigid body and the Euler Bernoulli beam.

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Modelling and Simulation in the Pulp and Paper Industry

USE OF MODELLING AND SIMULATION IN THE PULP AND PAPER INDUSTRY

ANGELES BLANCO, ERIC DAHLQUIST* , JOHANNES KAPPEN**,
JUSSI MANNINEN+, CARLOS NEGRO AND RISTO RITALA++
Chemical Engineering Department. Complutense University of Madrid, Spain.
*Mälardalen University, Vasteras, Sweden. **PTS, Munich, Germany.
+VTT, Espoo, Finland. ++Tampere University of Technology, Finland.

Corresponding Author: A. Blanco
Chemical Engineering Department, Complutense University of Madrid
Av. Complutense s/n, Chemistry Faculty, 28005 Madrid, Spain
Phone: + 34 91 394 42 47, Fax: + 34 91 394 42 43
email: ablanco@quim.ucm.es

The COST-Program is one of the oldest EU funded instruments to support the European scientific community. Hundreds of actions have been launched during the last decades, bringing together thousands of scientists. A action concerning modelling and simulation in the pulp and paper industry has been launched with a duration of 4 years. In pulp and paper the modelling of pulp production processes was the first big application. Since then several other applications have been realized though paper making has never been on the lead concerning the use of computer based modelling and simulation. The complex nature of the materials is one of the most demanding challenges and the biggest hurdle for any electronic description of the papermaking process or paper itself. So other industries took the lead and it is now for the paper industry to learn from these industries what can be done with the help of computers to control or optimise processes or to design new grades.

The main objective of the Action is to promote the development and application of modelling and simulation techniques in pulp and paper manufacturing processes. This is intended to eg. reduce emissions and increase the productivity and cost-efficiency of the processes. The main benefit will be a better understanding of the mechanisms of the processes and their control loops. This will help to find solutions for currently pending problems in the paper industry: improving the paper quality, optimising the wet end chemistry, enhancing the runnability and reducing emissions by improving process design, process monitoring and decision support during operation. In the long run this action should also contribute to designing superior or new product properties.

In this paper a review of the state of the art on modelling and simulation in the pulp and paper industry is presented as well as further research needs.

key words: modelling, simulation, pulping, papermaking.

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USE OF MATHEMATICAL MODELS AND SIMULATORS FOR ON-LINE APPLICATIONS IN PULP AND PAPER INDUSTRY

A. Avelin, J. Jansson and E. Dahlquist, Department of Public Technology
Malardalen University, Sweden

Corresponding Author: A. Avelin
Malardalen University, Box 883, S- 721 23 Vasteras, Sweden
Phone: + 46 21 101356, Fax: + 46 21 101370
email: anders.avelin@mdh.se

In this paper we discuss the accuracy of different types of models. First statistical models are discussed. They are built from process data and/or observations from lab measurements and are often called “black box models”.
Physical models which use physical relations to describe the process are using first principles and are often called “white models”. The third group of models is sometimes called “grey models”, as they combine the black box and the white models. Here we use basic physical principles but using statistical data from the process to tune the models. This can give a higher robustness than pure black box models as basic physics is included, but still the complexity of the models is not too high.

We give examples of different models. One statistical model was an ANN, Artificial Neural net. A boiler at Malarenergy in Vasteras was modelled to predict primarily NOx in the exhaust gases. Only already available data have been used to develop the “soft sensor” model. This example shows the difficulty with using statistical models without bothering about the process. It is so simple to get disturbing data or even noise built into a model, and it is actually quite difficult to see that this was done, if you rely on the statistical presentations of the model accuracy without considerations. In all cases we got the same statistical significance of the models, although we could judge that they were very different in reality, if we considered the real process physics! We also discuss PLS-models for paper properties from an integrated pulp and paper mill. This showed good correlation first, but lost accuracy by time.
The next example is a physical model of a continuous digester. The digester model includes mass balances, energy balances and chemical reactions and physical geometrical constants to copy the real digester. To make the digester model we have been using the program language Modelica.
We also discuss why there is no reason to have a more sophisticated model then motivated by the accuracy of the measurements.
The conclusion from the discussion about statistical and physical models is that a combination of them looks most attractive for the moment, and for the near future. Long term physical models becomes interesting when the computer power is significantly higher than today.

The question then arises how combined models should be performed. Our opinion is that we must start with understanding the process as far as possible. What is really taking place inside the process equipment? When we have identified what we believe is what is going on, a hypothesis should be made and models produced that takes into account this belief. The basic principles should be covered in a reasonable way and a few tuning parameters identified. These should both be relevant from a process point of view, and possible to determine from the process measurements or by manual sampling and laboratory analysis.

When this is done we have to consider how the process is operated. What variations do we have? What can happen that is out of our control, and can not be measured today? What changes do we have to control, like grade changes or production rate changes in the production? How can these dynamics be modeled?

Another question is how we can combine statistical models and physical models. Shall the statistical models be used to tune the physical models, or should they be used in parallel? How do we make use of the models for the on-line applications?

We will discuss these questions and try to formulate answers to at least some of them.

Optimal Pin Fin Heat Exchanger surface for Pulp and paper industry

H. Nabati and J. Mahmoudi, MDH, Västerås, Sweden;

Corresponding Author: H. Nabati
Dept. of Public Technology, Mälardalen University, MDH,
Västerås, Sweden
email:hamid.nabati@gmail.com

A large number of different heat exchangers are used in a pulp and paper mills. The pulp and paper industry consumes a noticeable portion of all the primary energy consumed in the industrial countries manufacturing.
Heat transfer enhancement in these heat exchangers could reduce the energy consumption considerably. Figure 1 shows a schematic diagram of a pulp and paper mill flow diagram.
Referring to heat exchanger behaviour in different conditions, the efficiency of the air-side heat transfer is a primary consideration when determining the best heat exchanger for a particular application. Furthermore, air-side heat convection is typically the limiting factor affecting heat performance of a heat exchanger. The convective heat transfer equation is proportional to surface area of the fins or bodies subjected to the airflow. Surface enhancement using pin fins could be a promising method of enhancing surfaces are in contact with the airflow. This study will focus on investigating the feasibility of HX performance improvement using pin-fin structures on the outer surface of the tube in pulp and paper industry. An optimal geometry will be suggested for the pin-fin design.
The goal of this study is to identify an optimal pin-fin surface for enhancement of air-side heat transfer. This research presents the results of numerical study of heat transfer in a Pulp and Paper heat exchanger, considering three different morphology pin fins(figure 2). A numerical study using Fluent software was conducted to select the optimum pin shape considering to maximize the heat transfer and minimize the pressure drop across the heat exchanger. The results indicate that the drop shaped pin fins yield a better treatment in heat transfer and pressure loss compared to the other pin fins. This improvement is mainly due to the increased wetted surface area of the drop pins, and the delay in the flow separation as it passes the more streamlined drop shaped pin fins.
This study also demonstrated that numerical models backed with experimental analysis can reduce both the time and money required to create and evaluate engineering concepts, especially those that deal with fluid flow and heat transfer in pulp and paper industry.

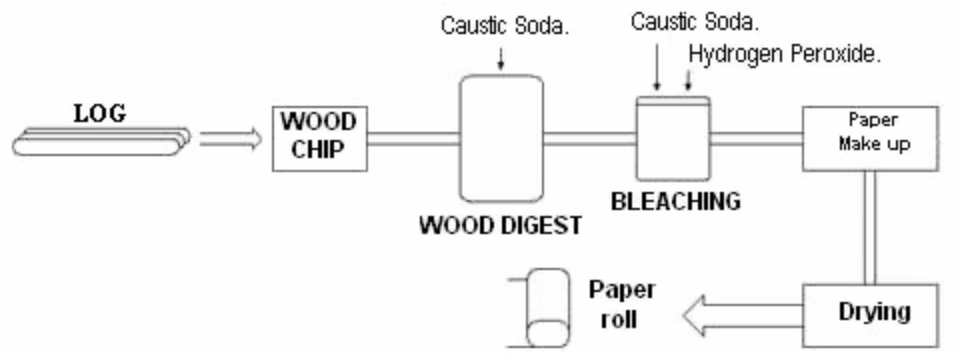

Figure 1: simplified process flow diagram of pulp and paper

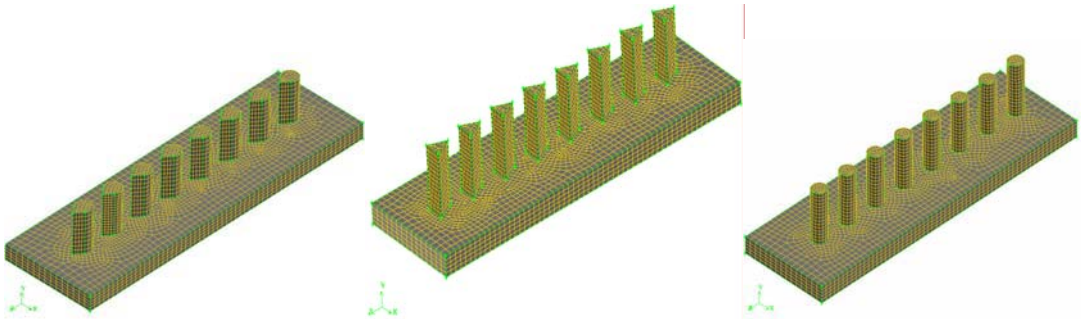

Figure 2: Different Pin-Fin sections as well as generated meshes

MODELLING OF UNCERTAINTY: CASE STUDIES ON OPERATION OF PAPERMAKING PROCESS

Heikki Jokinen, Kimmo Latva-Käyrä, Petteri Pulkkinen, Risto Ritala, TUT Tampere Finland

Corresponding Author: R. Ritala
Tampere University of Technology
P.O. Box 692, FIN-33101 Tampere, Finland
Phone: + 358 40 849 0922, Fax: + 358 3 3115 2171
email: risto.ritala@tut.fi

Operational decisions are influenced not only by the data and models available for the decision maker but also by the uncertainty in the data and model-based predictions on the impacts of decision makers' actions. In nonlinear systems the potential actions may have widely differing uncertainty associated with them. Then the decision maker must take an attitude towards risk and balance that against the expectation value of performance.

In stochastic optimization, methods to deal with uncertainty have been developed. There are several variants of the stochastic optimization problem: the utility theory, risk premium, optimizing expected performance under the constraint that probability of poor performance is below a given level, and minmax optimization. These formalisms have not been widely used in decision making about industrial processes. In this presentation, we present four slightly idealized cases, closely related to practical daily decision making tasks at paper mills: scheduling of pulp production under time-variant production costs, a grade change decision problem, optimization of the extent and frequency of laboratory measurements, and operation of a bistable biological water treatment plant. We formulate all these cases as decision making problems under uncertainty and express them mathematically within the frameworks of stochastic optimization. The level of description of the target system has been chosen realistic for the decision making task in question but such that it facilitates the simulation of the distributions of the variables directly, rather than requiring Markov Chain Monte Carlo (MCMC) simulations. The optimization problems are quite straight forward to solve and could thus be directly implemented at mills.

However, the difficulty in reality lies in that the methods expect that the decision makers' attitude towards risk is explicit and he/she can formulate the attitude through the parameters of the optimization problems, such as magnitude of risk premium or the highest acceptable probability of a poor performance to occur. According to our experience, the practical decision makers within industrial operation do not typically have a well-thought attitude towards risk, and even those that have face immense difficulties in expressing this attitude with the parameters of theory of decisions under uncertainty. We have also found the identification of the utility function through the gambling procedure too a complex approach for practical industrial operators. We propose that simulating optimal decision making at varied risk attitudes and consequent decision maker's trade-off between the resulting combinations of performance and risk is the main method of analyzing the decision makers' attitude towards the uncertainty and risk. In such an analysis the preferred combination of performance and risk corresponds to (not necessarily unique) risk attitude parameters. Once such parameters have been found, they can be taken in use in automated decision support, thus guaranteeing a consistent risk attitude. We discuss this approach in more detail when analyzing the operational decisions at the bistable biological water treatment plant.

Our conclusion is that the general theory provides a good ground for systemizing the risk analysis in operational and industrial decision making. We point out that this introduces new concepts to operational decision makers – operators and engineers – and thus is challenging to implement in practice. Furthermore, we note that present information and decision support systems do not support this approach.

Decision support systems (DSS) are an important category of manufacturing execution systems (MES). Decision making involves dealing with uncertainties and risk. In industrial circumstances measurements reduce uncertainty but as measurements are indirect some uncertainty will always be present. We suggest that the analytical approach towards decision making under uncertainty introduces a new paradigm for designing DSSs, and their data structures. The same approach yields also the value of measurements and how frequently they are repeated or supported with reference laboratory measurements.

APPLICATION OF ADVANCED DATA TREATMENT TO PREDICT PAPER PROPERTIES

A. Alonso, A. Blanco, C. Negro and J. Tijero, Complutense University of Madrid, Spain
I. San Pío, Holmen Paper Madrid, Spain

Corresponding Author: C. Negro
Chemical Engineering Department, Complutense University of Madrid
Av. Complutense s/n, Chemistry Faculty, 28005 Madrid, Spain
Phone: + 34 91 394 42 42, Fax: + 34 91 394 42 43
email: cnegro@quim.ucm.es

Papermaking is a process where there are numerous techniques and measurements to indicate paper quality. As the sector is becoming more competitive, a good control of paper quality is needed to assure users' requirements. This control can be carried out through paper properties predictions from different measurements from the process. However, paper properties predictions are not easy since during papermaking complex physico-chemical processes take place, especially in the wet end area. The flocculation mechanism produced in the wet-end will determine the floc properties during the formation of the sheet and, therefore, it will influence on retention, drainage and formation. Thus, it will affect the runnability of the machine and the properties of the final product. Due to the difficulty of predicting paper quality from wet end measurements the use of advanced data treatment is necessary. In this paper, Artificial Neural Networks (ANNs) have been used to predict paper properties from wet end parameters in a newsprint mill.

Process variables to be considered as inputs to the model have been selected according to previous experience at the mill and statistical analysis. In order to get additional information about flocculation, a focused beam reflectance measurement (FBRM) device has been installed on-line at the mill in the headbox. This device has been used to monitor flocculation following the methodology developed at the Complutense University [1-3]. This on-line methodology has been already applied in the fibre cement industry [4-5]. Results show that paper formation and strength properties can be robustly predicted from pulp properties, flocculation parameters and machine speed.

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Model Uncertainty and Control Consequences: a Paper Machine Study

Bernt Lie
Telemark University College, P.O. Box 203, N-3901 Porsgrunn, Norway, Bernt.Lie@hit.no

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Models are commonly used for prediction and design. All models are infected by model uncertainty, and it is thus of importance to have quantitative measures of how the model uncertainty influences e.g. model prediction capabilities.

Model uncertainties can be described in many ways. The study can be restricted to include parameter uncertainties under the assumption of structurally perfect models, or can be more realistic to include uncertainties in model structures. In general, it is difficult to describe uncertainties in the model structure. Parametric uncertainties can either be deterministic in that they are based on a physical understanding of the system under study, or they can be based on statistics, e.g. from model fitting.

Models are used extensively in designing control solutions. One possibility is to design a control input entirely based on the model, and then inject the computed control input into the system. This is often denoted *open loop* operation. Alternatively, a feedback (*closed loop*) solution can be developed, where for each time step, a control mechanism checks whether the real system operates as expected from the model. If the real systems drifts away from the response predicted by the model, a correction is introduced.

In this paper, deterministic and statistical descriptions of parametric model uncertainties are discussed, and illustrated with a case study from the paper industry. Prediction uncertainties under open loop and closed loop operation are then studied. The importance of taking advantage of the full model uncertainty description is stressed. With a naïve use of confidence regions, underlying correlations in parameters are not taken advantage of. It is shown how realistic parameter distributions can be found using the Bootstrap method.

The simulations of open loop and closed loop operation illustrate how a poor uncertainty description leads to uncertain predictions: even closed loop operation can not save a poor uncertainty description. The simulations also illustrate how the uncertainties can be reduced by using a proper uncertainty description, and how feedback (closed loop operation) will further reduce the system sensitivity to parameter uncertainties.

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Petrinets: Current Research Topics and their Application in Traffic Safety and Automation Engineering

Petrinets as a Concept for Modeling Transport Automation Systems

E. Schnieder, J. R. Müller

Corresponding Author: E. Schnieder
Technical University of Braunschweig
Institute for Traffic Safety and Automation Engineering
Langer Kamp 8, 38106 Braunschweig, Germany
Phone +49 (0) 531 / 391-3317, Fax: +49 (0) 531 / 391-5197
email: e.schnieder@tu-bs.de

In this paper we firstly identify the correspondences between the not formally but well distinguished concepts of system-theory and formal concepts of petrinet-theory and secondly trace the way from real world's things to models of theses things. Against this backdrop the area of transportation systems serves firstly to instanciate the abstractly defined system-theoretic concepts and secondly as the (real) outside world that is mapped to a (formal) petrinet-model (figure 1).

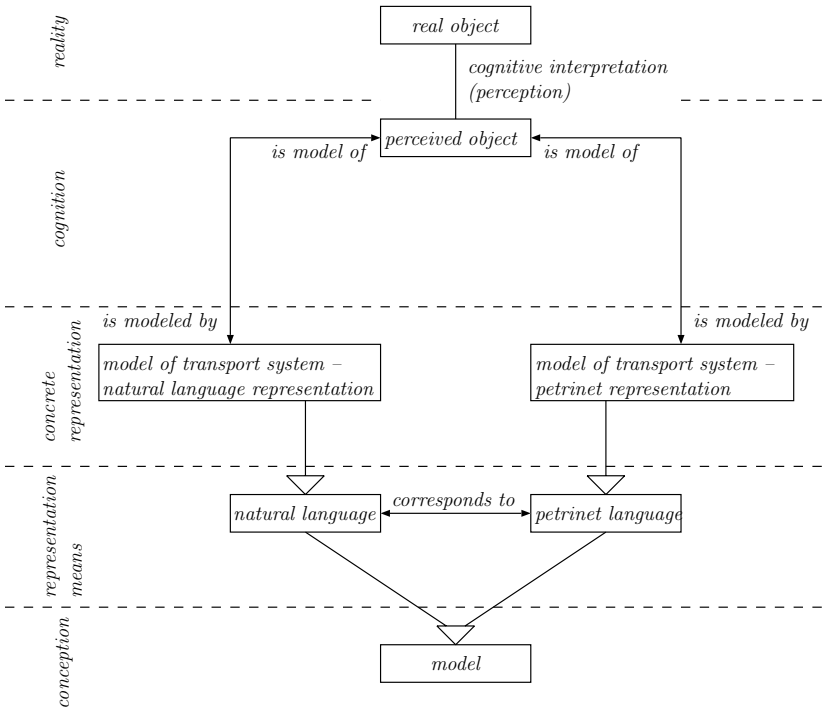

Figure 1: Relations between the real world, their perception and modeling

But why do we deal with system theory and petrinet-theory at all?
System theory serves with its concepts like *system-border, behaviour* and *emergence* as an instrument for the cognitive penetration of (circumstances of) systems as well as a plattform for the interdisciplinary discourse. With the help of system theory it is possible to question and if so to revise or to validate one's own individual perspective as well as to raise significantly the level of interdisciplinary discourses.

Although these concepts are well distinguished, a formalization to prevent ambiguouties and nondistinctives in discourses suggests itself. Because of it's attraction to scientists and engineers we use the formal language *petrinets* to formalize the fundamental concepts.

A PETRI NET APPROACH TO DEBUG SIMULATION MODELS OF LOGISTIC NETWORKS

P. Kemper and C. Tepper, Universität Dortmund, Germany*

Corresponding Author: P. Kemper
Universität Dortmund
LS Informatik IV, D-44221 Dortmund, Germany
e-mail: peter.kemper@udo.edu

Logistic Networks are the backbone of worldwide economies with high expectations in efficiency, performance and reliability. Model-based analysis in the design and management of Logistic Networks is an interesting application area for discrete event simulation.
In this paper, we describe how Petri net analysis techniques help to debug a large and detailed simulation model of airport logistics. The model is taken from a case study exercised in the field of air cargo networks and considers the flow of packets from starting airports to destination airports via two hubs. The focus is on the design of bundling procedures at hub airports and the goal of the study is to quantify the economic potential of different bundling strategies. The complexity of the resulting model turned out to be a challenge for validation, verification, and debugging, which is the topic of this paper.
The model itself is specified in the ProC/B notation, a simulation language that adopts the common process interaction approach. The ProC/B notation has been developed in particular to support modeling of logistic networks in a process-oriented manner. Large and complex models can be structured in a hierarchical manner based on the notion of functional units that provide services. The hierarchy is based on service calls and encapsulation of resources; each functional unit may contain own resources that are used to provide complex services. A resource may be a basic resource (active or passive) or a functional unit. This notion of hierarchy goes well with common structures in business organisations. So-called process chains in the ProC/B notation describe the potential behavior of different types of entities and the workload is generated by dynamic creation of entities during a simulation run. Entities formulate interacting processes with shared resources and those are likely to encounter partial deadlocks. For instance, allocation of multiple passive resources - counters in ProC/B terminology - are a prominent cause for deadlocks. In order to shed light on the role of resources and how they are used and allocated, we map the control flow of a ProC/B model to a Petri net and employ Petri net analyis techniques.
We describe a mapping that yields a Place/Transition net, such that we can apply invariant analysis. Since ProC/B models describe open systems with an unlimited number of entities, the resulting Petri net has an infinite state space and is unbounded. Invariant analysis helps us to recognize properties of a model or a submodel and to report those properties back to a modeller. By invariants we identify constraints among the different types of entities and we classify counters into reusable and consumable resources. For consumable resources, we check whether in case of simultaneous allocation of multiple resources, the allocation order is the same in all cases - a classical solution strategy for deadlock prevention. Furthermore, we identify simultaneous resource allocation for consumable and reuseable resources which needs extra attention to avoid deadlocks. The presented air cargo model has one configuration that allows for deadlocks due to an allocation of reusable and consumable resources in a particular submodel. Invariant analysis points us to the critical construction that causes the problem.
For that submodel, we can apply liveness and modelchecking to find a deadlock and generate an example trace that guides a modeller to the source of the problem. Clearly, liveness is only checked on a finite fraction of the state space. We achieve this restriction by considering the submodel in short-circuit with a limit on the number of entities. The crux of state-based analysis is the size of state spaces, the well-known state space explosion. In our case, we can apply two reduction rules (Berthelot's prefusion and postfusion rules) upfront to reduce the Petri net and retain its liveness properties. In the considered example, the reduction yields a Petri net with a state space that is reduced by several orders of magnitude. A subsequent liveness check identifies the deadlock and generates a trace to shed light on how it can be reached. After appropriate retransformation, the trace can be animated in the ProC/B toolset.
The overall approach is implemented within the ProC/B Toolset and partially makes use of the Petri net analysis methods implemented in the APNN Toolbox.

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CONSTRUCTION AND CORRECTNESS ANALYSIS OF A MODEL TRANSFORMATION FROM ACTIVITY DIAGRAMS TO PETRI NETS

Hartmut Ehrig, Karsten Ehrig, Claudia Ermel, Julia Padberg
Institut für Softwaretechnik und Theoretische Informatik
Technische Universität Berlin, Germany
email:{ehrig,karstene,lieske,padberg}@cs.tu-berlin.de

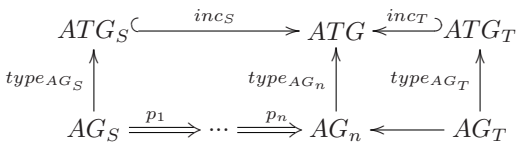
With the growing importance of model-driven development, the ability of transforming models into well-defined semantic domains becomes a key to automated analysis and verification in the software development process. In this paper we use the concept of typed attributed graph transformation to construct a model transformation from a simple version of activity diagrams to Petri nets. Our approach allows a correctness analysis which shows that this model transformation has functional behavior and is syntactically correct. This is the basis to use well-known analysis and verification techniques of Petri nets also for activity diagrams.

For the application of graph transformation techniques to visual language modeling, *typed attributed graph transformation systems* have proven to be an adequate formalism. Visual models given by typed attributed graphs can be manipulated by graph transformation rules. Roughly spoken a typed attributed graph transformation rule $p = (L \to R)$ consists of a pair of typed attributed graphs L and R (its left-hand and right-hand sides). A *direct graph transformation* written $G \overset{p,o}{\Longrightarrow} H$, means that the graph G is transformed into the graph H by applying rule $p \in P$ at the occurrence o of the left-hand side of the rule in G.

A visual language is modeled basically by an *attributed type graph* ATG_{VL} which captures the definition of the underlying visual alphabet, i.e. the symbols and relations which are available. Sentences or diagrams of the VL are given by attributed graphs typed over the type graph.

To be able to define a model transformation from a source VL S to a target VL T by graph transformation, the attributed type graphs ATG_S for the source language and ATG_T for the target language must be defined. Model transformation based on graph transformation is formally specified by a typed attributed graph transformation system $GTS = (ATG, P)$ consisting of an attributed type graph ATG and a set of model transformation rules P typed over ATG. Both type graphs ATG_S and ATG_T have to be subgraphs of type graph ATG. The model transformation starts with a graph AG_S typed over ATG_S. As ATG_S is a subgraph of ATG, AG_S is also typed over ATG. During the model transformation process the intermediate graphs are all typed over ATG. Please note that this type graph may contain not only ATG_S and ATG_T, but also additional types and relations which are needed for the transformation process. After the application of the model transformation rules P the resulting graph AG_n is typed over ATG, but not yet over the type graph ATG_T of the target language.

In order to delete all items in AG_n which are not typed over ATG_T we apply a restriction construction. The model transformation process is shown in the diagram to the right, where the data types for node and edge attributes are preserved during the process.



In our paper, we specify as source language simple activity diagrams, containing two kinds of symbol types, *activity* nodes and *next-relations* connecting two activities. Activities can be of different kinds, i.e. *simple* activities (inscribed by a name), *start* and *end* nodes as well as *decisions*. As the target language of our model transformation, we define an attributed type graph for elementary Petri nets. The model transformation rules map activities to transitions and next-relations to places in between. Decision activities are translated to two transitions, one for each decision branch. A sample model transformation is presented, transforming an activity diagram modeling a train dispatcher to a Petri net.

We analyse the model transformation rules with respect to the criteria *termination, confluence* and *syntactical and semantical correctness* and verify that the model transformation is correct and has *functional behavior* in the sense that the computed target model always is unique.

Integration of Planning and Production Processes

C. Simon, University Koblenz-Landau, Germany

University Koblenz-Landau
Institute for Management
Postfach 201 602, 56016 Koblenz, Germany
Phone +49 261 287 2861, Fax: +49 261 287 2851
email: simon@uni-koblenz.de

Motivated by the work of Ramadge and Wonham, in controller synthesis there is a major interest in states and the synthesis of state sequences to guarantee that forbidden states (unwanted or even dangerous situations) can always be prohibited. For the description of such systems, finite automaton and Petri nets are widely used. Both description languages have in common that the number of reachable states increases dramatically especially if some parts of a controlled machine perform independently from others. Because of the locality principle of Petri nets, they better support the representation of such independent components. Nonetheless, the number of represented states is effectively the same.
In computer science and information systems, state considerations are only one perspective on dynamic systems. Other perspectives are the data view and, increasingly important, the process view. This is motivated by the circumstance that since the work of Gaitanides, Davenport and Hammer and Champy organizational behavior is more and more considered as process driven (in opposite to a more functional structure of organizations which was - proposed by Kosiol - the predominant view since the 60ties). Hereby, business processes are well explained with languages like Event-driven process chains. Also here, Petri net approaches are widely used as for example Workflow nets. Process algebras, although supporting the proof of process properties, are not extensively used since they do not properly support visualization - a feature typically required by domain experts.
This paper introduces a Semantic Process Language which allows formally specifying and verifying process structures. The semantic of the words of this language are defined with the aid of Petri nets. As a by-product, a visualization of the processes is automatically given. Specific firing sequences of these Petri nets are then interpreted as the modules' processes. Figure 1 shows these concepts in a diagram.

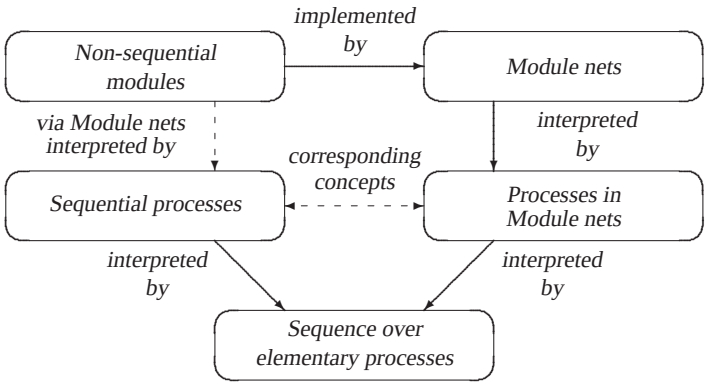


Figure 1: Relationship between the concepts of the paper

The paper does not only define the canonical implementation rules for modules in order to generate Petri nets out of them. It also demonstrates the use of this language for the verification of process properties on an abstract level which can then be applied to planning and production processes.

The Concept of Duality in Petrinets and it's Impact for Reliability Engineering

J. R. Müller, E. Schnieder

Corresponding Author: J. R. Müller
Technical University of Braunschweig
Institute for Traffic Safety and Automation Engineering
Langer Kamp 8, 38106 Braunschweig, Germany
Phone +49 (0) 531 / 391-3328, Fax: +49 (0) 531 / 391-5197
email: mueller@iva.ing.tu-bs.de

Abstract: Not only in automotive-industry new requirements concerning aspects related to costs, emission and performance of systems are reflected in serious challenges in model-based- and especially in model-based on-board diagnosis. A number of more or less formal methods have already been proposed, but these models have in common, that models for different fault cases are built often independently from the system's model.

The aim of this paper is to show that the theory of dual spaces can be brought in for (model-based) diagnosis. To do so, predicate/transition-nets are introduced, with arcs each labeled with a linear mapping as well as it's adjoint mapping (see figure 1).

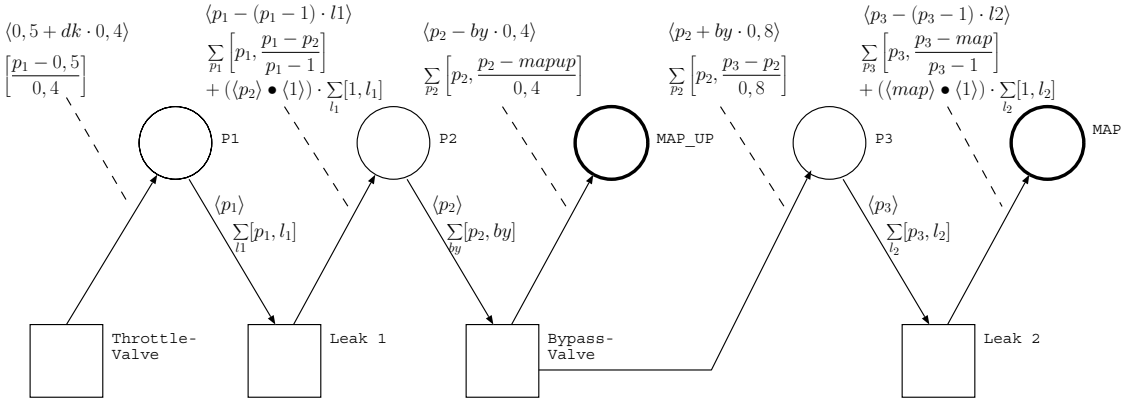


Figure 1: Pr/t-net model of the system to be diagnosed (a simplyfied airpath)

On the basis of such nets the space of possible faults (fault-space) is, starting at some observed values, successively narrowed down in a kind of fixpoint-calculation. Different observations at various working points lead to the calculation of different fixpoints (each representing a fault-space). Only the intersection of these spaces contains the fault-combinations consistent with all observations (see figure 2).

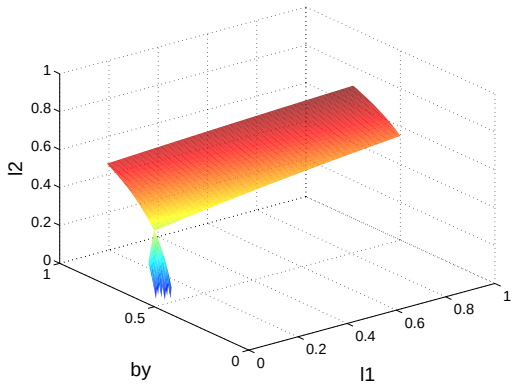


Figure 2: Two fault-spaces meet in exactly one point

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Modelling of Enviromental Systems

A FRAMEWORK DESIGNED FOR SOCIAL SCIENTISTS TO MODEL HUMAN AGENT BEHAVIOUR IN SOCIAL NETWORKS

Jochen Wittmann

University of Hamburg
Department for Computer Science, AB TIS
Vogt-Kölln-Straße 30, 22527 Hamburg, Germany
wittmann@informatik.uni-hamburg.de

Robert Tobias

Swiss Federal Institute of Aquatic Science and Technology, SIAM
Überlandstrasse 133, 8600 Dübendorf, Switzerland
Robert.Tobias@eawag.ch

Abstract

In the context of applied psychology modelling human behaviour is intensively discussed. There are various psychological theories that focus on psychological aspects of decision making and on communication aspects. It is obvious to analyze these questions by the means of modelling and simulation. In this situation, the modeller has two main problems: Firstly, there are lot of very detailed investigations on psychological phenomena but all these theories are quite isolated to each other and do not give an integrated and comprehensive view on the relevant process. Secondly, for formulating the model and for simulating it later on, there is no support on software level.

In this situation an efficient software concept is needed which brings together the very special objectives of the innovative and continuously developing thematic scope and a scalable and payable software architecture to work with. This paper introduces such a software concept. Preconditions for the work are a communication network simulator and a psychological model for a human agent. The network enables the modeller to specify communication networks between the modelled individuals, the agents and executes a simple next-event-simulation mechanism with a discrete time-model. The agent model structures the psychological components and processes participating in decision making.

The main part of the paper analyzes the use cases for the planned software system as initialize the network, initialize an agent, observe trajectories, simulate, analyze results, change parameter values, change agent behaviour, and focuses on the special problems caused by applying these tasks to the field of agent based communication models. On the base of these deliberations an adequate software architecture is proposed. Thereby, the following conflicts had to be solved:

- Complexity of the model versus design of the user interface.
- Universal software system versus easily adaptable simulation program.
- User interface versus highly specialized interventions on behaviour programming level.
- Object oriented programming paradigm versus (procedural) programming skills of the social scientists.

These conflicts concentrate on a cost benefit problem concerning universal system and comfortable user interface on the one hand and on the problem of the access level for the inexperienced user on the other. The decisions made for models following the ATASIS meta model are as follows: The graphical user interface gives support only for simple standard functions. Higher functionality is accessible by the interface of the database system and its query language directly. For the model description level the argumentation is more complex. The solution is realized as follows:

1. Model structure in strong analogy to the psychological theory.
2. Strongly sequential runtime algorithm.
3. Dataflow by message mechanism between the psychological components.
4. Updating the model code by the use of a standard development environment.

So far, the conflict between a proper object-oriented design of the modelling and simulation software environment for the ATASIS meta model and the usability by users without deepened programming skills is discussed. For the complete project of model development, this paper tries to motivate

- A sophisticated balance between user skills and higher concepts of object oriented programming paradigm: We just used the concepts of modularisation but no heritage and no method concepts.
- The cost benefit calculations for the user interface, which lead to very pragmatic solutions especially for non standard application areas of simulation methodology.
- The intensive analyse of user demands which leads to smaller and more efficient solutions.
- The concept of the expert-mode interface for access to model code and data base which leads to an open system architecture with only negligible cut backs in comfort.
- The acceptance and integration of user skills which has restricting effects concerning programming experiences however very positive effects concerning the use of the database interface including its query language.

EXPERIMENTAL DESIGN FOR AGENT-BASED MODELLING APPROACHES

Jochen Wittmann, University Hamburg, Germany

University Hamburg, Department for Informatics, AB TIS
Vogt-Kölln-Straße 30, 22527 Hamburg, Germany
email: wittmann@informatik.uni-hamburg.de

Abstract

The object oriented modelling paradigm has established during the last years and leads especially for the application areas biology, sociology to its specialization in the form of so called „individual-based“ models. This paper will neither discuss the definition problem (What is an “individual-based” model?) nor the model building process. It will analyse the validation step during a simulation study for the case an individual-based approach has been chosen. With regard to the main application areas of individual-based models, which mainly are applied in domains without exact physically derived model descriptions, this important phase in a simulation study attracts special attention.

To understand the problems concerning validation, the paper starts with a view on the general design of a modelling and simulation study based on the individual-based paradigm. It postulates that input data, model and model output are on the same aggregation level (accumulated data for differential equation models on the one hand and individual data and individual based model description on the other).

The problems arise, if there are changes in aggregation level in the argumentation line of a simulation experiment. Doing so, transformations between the individual based level and the aggregated level become necessary. Usually, these transformations are evident and easily to execute. However, to additional assumptions have to be made concerning the transformation function: Mostly it will be a statistical hypothesis associated with two additional parameters that have to be considered carefully:

1. the type of distribution of the parameter transformed (e.g. uniform, normal, ...)
2. parameters of the distribution, such as mean value, variance, ...

These parameters have to be determined and they influence the experimental design substantially: In the first case, the model results are independent of these transformation parameters, in the second case there is a proper distinction necessary between the influence and effects of the transformations and their parameters and the effects of a change in the model parameters which in fact are under observation to achieve the experiments objectives.

In this situation the paper proposes four typical settings for experimentation with individual based models, explains their structure, identifies the corresponding validation and interpretation problems, and gives hints for correct experimental design and argumentation. The four settings are:

1. The focus of the observation lies on investigations on individual behaviour.
2. The intention to use structural adequate models as description for processes on the global/accumulated level.
3. Necessary measurements are not possible on the desired level of abstraction and/or model description.
4. Investigations concern the phenomena of emergent behaviour.

To conclude, the last section of the paper discusses the four design templates for the well known predator-prey model and illustrates the problems and the argumentation for the different experimental set-ups.

The example leads to the conclusion that each transformation between modelling levels has additional parameters for its own that normally have to be determined by additional statistical experiments.

A comparison of results gained by models on the different levels may be interesting, however, its statistical value for validation and interpretation of possibly appearing effects is negligible.

The proposed scheme does not provide an algorithm to solve the problems in using individual-based models but it tries to make the typical structures of argumentation using such models transparent and tries to give a guideline for the discussion of critical aspects and common problems using these types of models.

OPTIMISED CONTROL OF ADAPTIVE CURRENT CONSUMERS – A FIRST APPROACH

U. Vogel, J. Pei, M. Sonnenschein, Univ. Oldenburg, Germany

Corresponding Author: U. Vogel,
University of Oldenburg, Dept. of Computing Science
Uhlhornsweg 84, D-26111 Oldenburg, Germany
Phone: +49 441 798 2752, Fax: +49 441 798 2756
email: ute.vogel@informatik.uni-oldenburg.de

Conventional methods for producing electrical energy from fossil fuels or nuclear energy depend on limited resources. So, experts recommend the transition to renewable energies. One mayor drawback of most of these renewable energy sources is their temporal availability: the power supply of solar energy electric power stations and wind power converters e.g., depends on weather conditions and hence is fluctuating. So, the possible gap between the temporal varying demand for energy and the energy supply is intensified. Bridging this gap by short-time controllable power plants is very expensive. For this reason, energy suppliers are interested in smoothing the peaks in the difference between supply and demand.

Our approach in this paper is to explore the possibilities of shifting the consumption of electrical energy with respect to a prognosis of energy availability for a fixed time interval.

Many energy consuming tasks are not bound to be started at a certain point of time. Often it is sufficient, if these tasks are fulfilled in a given time interval. So, throughout this paper, we will consider such tasks as "jobs" $j = (a(j), e(j), d(j), m(j))$, which are characterized by an earliest starting time $a(j)$, a latest due time $e(j)$, $a(j) \le e(j)$, a duration $d(j)$, and an amount $m(j)$ of energy, which must be supplied for the duration of the job.

As the power supply of wind energy converters can be predicted with acceptable precision for time intervals of about 24 h in advance, we assume for a time interval T that the energy supply is a known function $C: T \rightarrow \mathbb{R}$.

The problem is now to find a choice $(x(j))_{j \in J} \in \{0, 1\}^{|J|}$ of the given set J of jobs and starting times s(j) for these jobs which guarantees that each job is performed during its allowed time interval [a(j), e(j)], and that at each time t during the time interval T the energy demand $B(t) = \sum_{s(j) \le t \le s(j) + d(j)} m(j) \cdot x(j)$ does not exceed the energy supply C(t). The optimal solution is a solution (x, s) which also maximizes the allocated amount of energy $\sum_{j \in J} d(j) \cdot m(j) \cdot x(j)$. This basic problem is NP-hard. As realistic applications afford that every job has to be performed, we experimented with a more realistic model that schedules all jobs and minimizes the difference between power supply and demand. Due to the temporal fluctuating availability of the single resource, this problem can not simply be transformed to a conventional scheduling problem.

As a first approach for determining a solution of the given optimization problem, the well-known meta-heuristic Tabu Search was investigated [2, 3]: We set up the neighbourhood function suitable to our problem and experimented with ten different instantiations of Tabu Search, in order to find the best parameters and instantiation. Using five randomly generated test cases, which consist of about 3500 different sets of jobs, we analyzed the behaviour of these Tabu Search instantiations.

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TIME SERIES MODELLING OF WATER QUALITY INDICATORS

Jean Duclos Alegue, Albrecht Gnauck, BTU Cottbus, Germany
Corresponding Author: J. D. Alegue
Brandenburg University of Technology at Cottbus
P.O.B. 10 13 44, D-03013 Cottbus, Germany
Phone +49-355-692713, Fax +49-355-692743,
e-mail: jeduclo@yahoo.com

Freshwater resources, on which human life depends, are presently facing accelerating rates of degradation especially in developing countries. Human health is significantly affected in this process. While the water-crisis is well known in areas such as the Middle East and some parts of Africa, a good number of water professionals believe that freshwater quality will in future become the main limiting factor in sustainable development in many countries (Ongley, 1999).
In order to assess the quality of water resources as well as water quality policies, chemical, physical and biological variables are recorded over time by monitoring programs. These variables give information on the current status, the changes and trends in water quality. The measurements obtained depend on both natural and anthropogenic processes. Fluctuations from the mean value over time can be as a result of parallel acting internal and external driving forces. Seasonal and periodic processes influence the fluctuations causing water quality indicators to portray a cycling behaviour over time. The patterns displayed by these variables can be captured and used for forecasting by means of appropriate modelling techniques. The models give more insight to the time behaviour and internal correlation structure of the indicator. They are also quite helpful for comparing standards and methods of standardisation in and between regions.
The Fourier polynomial is a technique for approximating periodic functions by sums of cosine and sine periodic functions, shifted and scaled. It may therefore be suitable for approximating cycling processes. Physical, chemical and biological water quality indicators from the Havel River at Potsdam were modelled using this technique.
The models for physical indicators such as water temperature had a coefficient of determination above eight, and below eight for the biological indicators and below six for the chemical indicators. This is because a physical indicator like water temperature is mainly influenced by external driving forces such as solar radiation while high fluctuations observed in biological indicators like chlorophyll-a are dependent on external driving forces and internal ecological state variables such as light and nutrients availability. Chemical indicators such as dissolved oxygen are significantly influenced by natural and artificial externakl driving forces as well as by natural internal states. They fluctuate as these factors fluctuate. In addition, because the Fourier polynomial is appropriate for processes with fixed frequencies while natural processes have varying frequencies. The results of the ongoing investigations on the use of digital filters and artificial neural network for modelling water quality indicators will be presented with time.

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MODELLING OF PHOSPHORUS CHANGES IN A SHALLOW RIVER-LAKE ECOSYSTEM

Albrecht Gnauck, BTU Cottbus, Germany
Corresponding Author: A. Gnauck
Brandenburg University of Technology at Cottbus
P.O.B. 10 13 44, D-03013 Cottbus, Germany
Phone +49-355-692713, Fax +49-355-692743,
e-mail: umweltinformatik@tu-cottbus.de

Sustainable management decisions to control freshwater ecosystems can only be achieved by using powerful simulation tools. The functioning of ecosystems and various water uses will be affected by polluted water. Pollution refers to intensive man-made activities in a river catchment which result in an ongoing eutrophication process in lakes. This process is characterised by increasing concentrations of dissolved nutrients, by excessive growth of plants, mainly algae, and by restricted water uses due to anoxic water conditions as well as by odor problems, and risk human health. In shallow water bodies internal pollution by nutrient remobilisation from sediment plays an important role additionally. To forecast the nutrient dynamics in shallow lakes a simulation framework for a subcatchment of the River Havel was worked out (Gnauck et al. 2003).

For the process of internal pollution due to phosphorus remobilisation from sediment a submodel was added to the eutrophication model *HavelMod*. State variables are phytoplankton and zooplankton, orthophosphate phosphorus and nitrogen compounds as well as dissolved oxygen and biochemical oxygen demand. Photoperiod, solar radiation and water temperature are used as external driving forces. The eutrophication model itself consists on nine differential equations. It was carried out within the MATLAB environment.

To get optimal management proposals the eutrophication simulator *HavelMod* was combined with the software tool ISSOP (Krug 2002). It includes multicriteria optimisation procedures of MATLAB models. For coupling of *HavelMod* and ISSOP an open interface was used. ISSOP uses the model variables and target values as input data and gives back optimised state variables to the simulation system.

The coupled software tool was applied to a stretch of the Lower Havel River with time series of water quality data from 1997 as references. The optimisation problem was solved by using gradient search method combined with MCM. For water quality management two alternatives are taken into account: Eutrophication control according to the limiting nutrient concept of algal biomass (Uhlmann 1975), and according to LAWA (1998). As a result, an eutrophication control according to the limiting nutrient concept leads to a diminished phytoplankton maximum in late summer by optimised nitrate concentration. No effect of optimised orthophosphate phosphorus concentration can be stated. On the other hand, control according to target values of LAWA leads to nearly the same behaviour in spring but to a smaller difference of phytoplankton maxima in late summer.

Perspectives of simulation frameworks for water quality management on a river basin scale may be seen in combinations of water quality simulation models, optimisation procedures and visualisation tools.

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Optimzation in Multibody Dynamical Systems

OPTIMISATION OF CVT ROCKER PIN CHAINS

Friedrich Pfeiffer, Heinz Ulbrich, Lutz Neumann, TU München, Germany

Corresponding Author: Friedrich Pfeiffer
Lehrstuhl für Angewandte Mechanik, TU München
Boltzmannstraße 15, 85748 Garching, Germany
email: Pfeiffer@amm.mw.tum.de

Continuous variable chain drives have to satisfy high requirements to compete with common gears and therefore an improvement of certain properties of the CVT (= Continuously Variable Transmission) is desired. In this contribution the important goal to reduce the noise emission of the gear is realised by optimising the geometry of the rocker pin chain. This optimisation is carried out by applying numerical simulation techniques and an optimisation algorithm.

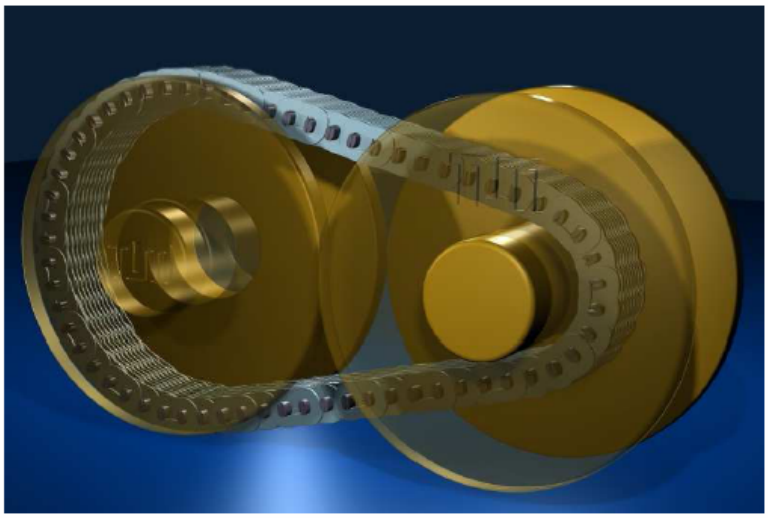

Figure: Simulation Model of the CVT

For this purpose a detailed dynamical model of the CVT is introduced which includes an exact treatment of the rocker pin kinematics of the chain. The geometry of the rocker pin joints which shall be optimised is defined by the optimisation parameters. A good choice for a measure of the noise emission is the amplitudes of the forces in the bearings in a certain frequency domain. They are used to form the target function. A numerical simulation provides a connection between the optimisation parameters and the objective function, which is not given analytically and takes high simulation effort.

Therefore the optimisation algorithm *implicit filtering* is applied to solve the optimisation problem. The presented approach is applied to minimise the noise emission of a CVT by finding optimal geometry parameters. A significant reduction of the noise emission is gained. The optimisation can be carried out on standard PCs.

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OPTIMAL MOTIONS OF CERTAIN MUTIBODY SYSTEMS IN RESISTIVE MEDIA

F.L. Chernousko

Institute for Problems in Mechanics of the Russian Academy of Sciences
101-1 Prospect Vernadskogo, Moscow 119526, Russia
Phone: +7-095-4340207, Fax: + 7-095-9382048
email: chern@ipmnet.ru

Various non-conventional principles of motion of multibody systems in resistive media are considered. These principles do not imply using wheels, legs, tracks, screws, propellers, jets, and other devices and are based on relative motions of some parts of the moving bodies in the presence of external resistance forces. Namely, two kinds of motions are investigated:

- snake-like locomotion of multilink systems;
- progressive movement of a body caused by internal motions of a mass inside this body.

Both types of motion are possible only in the presence of external resistance forces such as Coulomb's dry friction or viscous resistance.

For the snake-like locomotion, multilink mechanisms equipped with actuators installed at the joints are considered. The mechanism can move along a horizontal plane in the presence of Coulomb's dry friction between the mechanism and the plane. The locomotion is a result of periodic twisting of the mechanism at its joints controlled by the actuators. For two-link and three-link systems, these periodic motions consist of alternating slow and fast phases. Multilink mechanisms with more than four links can perform smooth wave-like locomotion.

Optimal geometrical and mechanical parameters of the multilink mechanisms as well as optimal parameters of periodic motions are obtained that maximize the average speed of locomotion. The optimization is carried out numerically. It is shown that the optimization leads to a considerable gain in the locomotion speed. The results of optimization are compared with the experimental data. The results of computer simulation, animation and videofilms are presented.

Another kind of motion is caused by a periodic displacement of a certain mass inside the moving body. Here, various types of external resistance forces are examined: Coulomb's dry friction, linear and quadratic resistance forces depending on the velocity of the body. Both symmetric (isotropic) and asymmetric (anisotropic) cases of resistance are considered; in the latter case, the resistance forces for the forward and backward motions of the body are different.

Optimal relative periodic motions of the internal mass are obtained that result in the maximum average speed of the moving body. The analytical and numerical results of the optimization and videofilms are presented.

The obtained results are of interest with respect to mobile robotic systems, especially, for mini-robots.

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Discrete-Time Control by Nonlinear Online Optimization on Multiple Shrinking Horizons for Underactuated Manipulators

Dirk Weidemann†, Norbert Scherm‡, and Bodo Heimann†,

† Hannover Center of Mechatronics
University of Hannover
Appelstraße 11, D-30167 Hannover, Germany
Email: {weidemann, heimann}@mzh.uni-hannover.de
‡ Institute of Automatic Control
University of Hannover
Appelstraße 11, D-30167 Hannover, Germany
current address:
Rheinmetall Defence Electronics
Brüggeweg 56, D-28305 Bremen, Germany
Email: scherm.n@rheinmetall-de.com

Discrete-time controllers based on an extended linearization perform well for different kinds of underactuated systems such as highly underactuated manipulators or cartpole systems if the trajectory deviations are small. In order to counteract large trajectory deviations, a discrete-time feedback controller for underactuated manipulation systems based on nonlinear online optimization is proposed in this paper. To reduce the computation time, an initialization strategy of the nonlinear online optimization is presented considering the relation between the feedback controller based on nonlinear online optimization and a feedback controller based on extended linearization. The proposed feedback controller is applied to a 2-DOF underactuated manipulator with a passive joint operating in the horizontal plane. Experimental results are reported to demonstrate the efficiency of feedback control by nonlinear online optimization.

The paper is structured as follows. The dynamics of the underactuated manipulator and the discrete-time notation are given in Section 2 and Section 3. In Section 4 the feedback controller based on an online optimization is presented. The experimental results are given in Section 5.

Although a feedback controller based on an extended linearization shows good performances for several underactuated systems, it is only valid for small errors. In this paper, a feedback controller based on a nonlinear online optimization has been proposed. The aim of the latter feedback controller is to overcome the disadvantages of a feedback controller based on an extended linearization. The relation between the controllers based on online optimization and on extended linearization is used to derive an initialization strategy for the online optimization. In contrast to most model predictive control strategies a shrinking horizon approach has been applied to fully utilize the relation between both feedback controllers. Finally, experimental results have demonstrated that the feedback controller based on a nonlinear online optimization is more suitable to reduce large initial errors than a feedback controller based on an extended linearization.

OPTIMAL CONTROL OF SHOCK ISOLATION SYSTEMS ON THE BASIS OF THREE-COMPONENT MODELS

D.V. BALANDIN, Nizhny Novgorod State University, Russia, N.N. BOLOTNIK, Institute for Problems in Mechanics of the Russian Academy of Sciences, W.D. PILKEY, University of Virginia, USA, and S.V. PURTSEZOV, University of Virginia, USA

Corresponding Author: N.N. Bolotnik
Institute for Problems in Mechanics of the Russian Academy of Sciences
101-1 Prospect Vernadskogo, Moscow 119526, Russia
Phone: +7-095-4343292, Fax: + 7-095-9382048
email: bolotnik@ipmnet.ru

This paper contributes to scientific foundations of the optimal design of shock isolation systems. The optimal design involves the limiting performance analysis aimed at the determination of the absolute minimum of a numerical criterion measuring the operating quality of the system. The knowledge of this minimum enables the designer to assess the quality of the existing systems and prospects for their improvement. The design configuration is not taken into account at this stage and the shock isolator is regarded as a generator of the force between the object to be protected and the base subject to a shock disturbance. This force is treated as the control variable and the limiting performance analysis is reduced to an optimal control problem. A comprehensive presentation of the limiting performance concept is given in [1, 2].

In most publications on the optimal control of shock isolation systems, a two-component model involving the object to be protected and the base is utilized. However, such a consideration can be inadequate in a number of cases, in particular, when dealing with the design of shock isolation systems for transport vehicles. In this case, more adequate is a three-component model that involves the object to be protected, the container to which the object is attached by a shock isolator, and the base, which can be attached to the base by an additional shock isolator. In specific systems, the role of the base, the container, and the object can be played by rather different bodies and structures. For instance, for an aircraft, the landing gear carriage can be regarded as the base, the fuselage as the container, and the passengers as objects to be protected. The seat cushions play the role of isolators between the fuselage and the passengers and the landing gear shock absorber can be treated as an additional isolator between the carriage and the fuselage. In modern crashworthy passenger cars, the impact isolation of occupants of the car from a frontal crash impact is provided not only by the restraint system (seat belts and airbags) but also by appropriate deformation properties of the front part of the car. In this case, the role of the base, the container, and the object is played by a front panel of the car body, the compartment (cabin), and the occupant, respectively. The seat belt and the airbag can be regarded as the isolators between the object and the container, and the deformable portion of the car front end as the additional isolator between the base and the container.

We propose a technique for the shock isolation limiting performance analysis on the basis of the three-component model. This involves the solution of an auxiliary problem for a two-component system. The two-component system involves only the base and the object to be protected. In addition, the auxiliary problem involves only one control function – the control force acting on the object, whereas the primary problem has two control functions – the control force acting on the object and the control force acting on the container. This makes the auxiliary control problem easier to solve. Having known the optimal control and the minimum of the performance index for the auxiliary problem, one can determine the optimal controls and the minimum value of the performance index for the primary problem for the three-component system. The solutions of these two problems are related by simple analytical equations.

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ROBOT PLACEMENT IN A PRODUCTION CELL

K. Gotlih, UNI Maribor, Slovenia

Corresponding Author: K. Gotlih,
University of Maribor, Faculty of Mechanical Engineering
Smetanova 17, 2000 Maribor, Slovenia
Phone: +386 2 220 7961, Fax: + 386 2 220 7990
email: gotlih@uni-mb.si

Robots are, in many cases of modern production cells, used as manipulation devices, as manufacturing machines or as measurement systems. Today a production cell is designed mostly for high capacity serial production of some well-known product.

In the designing phase of the production cell, whenever the use of robots is planned, some important questions appear:

- Which mechanism configuration will fit the requirements best?
- How fast the production cycles are and whether the robot is able for that or not?
- Does the robot's configuration space cover the required task space in the production cell with required quality?

Some answers to these questions can be obtained when the production cell is designed and simulated with some commercial available software systems. These simulation software systems mostly assure collision avoidance of the robot with its environment. The placement of the robot mechanism into the cell is still done on the basis of designer's experience and intuition. The covering of the task space in the production cell with the configuration space of the robot is still unanswered at this point.

The subject of this paper is to show a part of a research work where we try to find an appropriate tool for defining the robot's location in the production cell according to requirements. This location should assure the covering of the required task space with the robot's configuration space and guarantee the best possible performance of the robot in each point of the task space.

The performance of the robot in a point of the task space is defined with the smallest singular value of the robot's Jacobian matrix in that point. The smallest singular value in a point of the task space is proportional to the shortest axes length of the velocity ellipsoid in the observed point. The shortest axes length of the velocity ellipsoid and its direction indicate the smallest possible velocity of the tool centre point and its direction in the observed point. In other words the tool centre point cannot move faster in the direction of the shortest ellipsoid axes as it is indicated with axes length. The position of the robot's base relative to the task space is obtained with an optimisation. The mathematical formulation of the optimisation procedure is written in the statement:

$$min(\frac{1}{n_{po\,int}}) \qquad \textit{with respect to}$$

$$x_{i,min} \le x_i \le x_{i,max} \qquad i = 1, n \qquad \textit{and a non-linear constraint}$$

$$n_{min} \le n_{po\,int} / n_{poall} \le n_{max}$$

The design parameters x_i, $i = 1, n$, are the coordinates of the task space origin with respect to the robot's base origin. $n_{po\,int}$ is the number of points in task space which satisfy $\sigma_n \ge \sigma_{tres}$. σ_n and σ_{tres} are the smallest scaled singular value of the Jacobian matrix and the threshold value which is prescribed. n_{poall} is the number of all points in the task space. The non-linear constraint $n_{po\,int} / n_{poall}$ is responsible for forcing the task space origin to a point where the difference between the numbers of all points n_{poall} in task space is small in relation to the number of points $n_{po\,int}$ with $\sigma_n \ge \sigma_{tres}$.

To illustrate the described procedure a SCARA robot mechanism with 2 degrees of freedom is chosen. In the presented example the number of feasible points increase dramatically from 1004 for the initial position of the task space to 1960 points in the optimal position of the task space. The covering of the task space is almost complete (97%).

OPTIMIZATION OF RAIL WHEEL PROFILES

R. Kovalev, TU Bryansk, Russia

Corresponding Author: R. Kovalev
Bryansk State Technical University
bul. 50-let Oktyabrya 7, 241035 Bryansk, Russia
Phone, Fax: +7 4832 568637
email: kovalyov@tu-bryansk.ru

Shape of railway wheel and rail profiles strongly influence on performances of contact interaction, dynamical performances of a railway vehicle as well as on fatigue and durability of railway vehicles and track. Optimization of railway wheel and rail profiles is considered as the most effective way for improvement interaction between railway vehicles and track.

Shape of railway wheel profiles is the subject that has been discussed during all the time railway vehicles exist. In the beginning railway wheels were cylindrical, then became conical for better guidance and now they usually have complex profiles. Dynamical performances of railway vehicles especially wear, stability and safety significantly depend on shape of wheel profiles. The main difficulty of the problem consists in contradictoriness of the criteria: the better wear factor the usually worse the stability and correspondingly the safety.

A strategy for railway profile optimization is suggested. An example of implementation of this strategy to wheels of freight wagons is shown.

Objective function includes the following criteria: track loading, stability in tangent tracks, wear factor in curves, derailment quotient, and contact stresses.

Calculation of the objective function is based on results of numerical simulation. The commercial software package Universal Mechanism is used for simulation of rail vehicle dynamics. The procedure for synthesis of the wheel profiles using the vector of parameters was incorporated into Universal Mechanism.

In order to take into account basic operating conditions of freight cars each profile is tested using the following conditions:

- car type (open wagon and hopper);
- loaded and empty car;
- curves and tangent tracks;
- degree of wear of external rail profile (new rail profile and side wear 4 and 8 mm).

The Universal Mechanism software has a built-in service of distributed calculations, which allows using any computer reachable by the TCP/IP communication protocol for parallel numerical experiments. Using the service of distributed calculations within the Laboratory of computing mechanics at Bryansk State Technical University (8 personal computers, 600 MHz – 2.4 HHz) gave us a possibility to analyze up to 1500 wheel profiles a day. Totally about 6000 railway profiles were estimated during the phase of preliminary analysis. Usage of only one computer would took about 20 days to fulfill such the set of experiments.

Obtained optimal wheel profile joins relatively small wear factor and quite safe derailment quotient that seems to be quite promising result.

This work has shown that the suggested optimization strategy produces promising results and can be used for optimization of the wheel profiles. The strategy considers typical operating conditions including tangent tracks and curves and various rail profiles.

Further investigations assume testing optimal wheel profile as well as development of the improved strategy that could predict and involve changing a shape of a profile during operations.

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Optimal Control of Applications described by DAEs/PDEs/PDAEs

Modeling of an MHD Free Surface Problem Arising in CZ Crystal Growth

R. Griesse, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria
A. J. Meir, Department of Mathematics and Statistics, Auburn University, USA

Corresponding Author: R. Griesse
Johann Radon Institute for Computational and Applied Mathematics
Austrian Academy of Sciences
Altenbergerstraße 69, 4040 Linz, Austria
e-mail: roland.griesse@oeaw.ac.at

In this paper we consider some aspects concerning the mathematical modeling of free surface problems arising in technical processes which involve the interaction of electrically conducting fluids and magnetic fields, described by the equations of magnetohydrodynamics (MHD). To focus the discussion, we restrict ourselves to the Czochralski (CZ) process in crystal growth. The CZ crystal growth process is used, for instance, to grow silicon crystals for the semiconductor industry. The silicon is melted inside a crucible before a seed is lowered into the melt to initiate the crystallization process. The seed is slowly pulled upwards, and the pulling speed determines the diameter of the ingot. A schematic of the CZ process is shown in Figure 1.

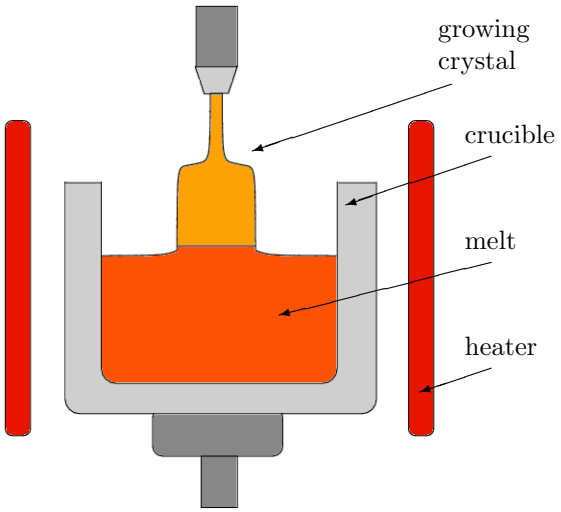


Figure 1: Schematic of the CZ process and geometry of the free surface problem.

Due to temperature gradients in the hot melt, a strong buoyancy-driven flow can develop. On the free surface, the surface tension and its variation with temperature also drives fluid motion, known as the Marangoni effect. In addition, both the seed and the crucible are often rotated. Rotating or steady magnetic fields may be applied to influence the fluid motion in a favorable way. Some of the concerns are non-uniform dopant distribution and impurity striations. The goals include the reduction of radial and axial temperature gradients and a flow field close to an axisymmetric configuration, in order to homogenize solute concentration. In addition, it is desired to damp out flow instabilities, or to overpower turbulence which otherwise lead to deterioration of the final crystal's properties.

The current work differs from prior work in a number of aspects. One main feature of the model presented is the use of the electric current density rather than the magnetic field as the primary electromagnetic variable. Here the induced magnetic field is recovered from the current density via the Biot-Savart law making idealized or artificial electromagnetic boundary conditions unnecessary. This allows us to account for the interior and exterior magnetic fields even though the equations are posed on the (bounded) fluid and conductor regions. In addition, we do not assume that the flow is two-dimensional but allow for fully three-dimensional flows.

A NONSMOOTH NEWTON'S METHOD FOR CONTROL-STATE CONSTRAINED OPTIMAL CONTROL PROBLEMS

M. Gerdts, University of Hamburg, Germany

University of Hamburg
Bundesstrasse 55, 20146 Hamburg, Germany
Phone: +49 40 42838 5112, Fax: +49 40 42838 5117
email: gerdts@math.uni-hamburg.de

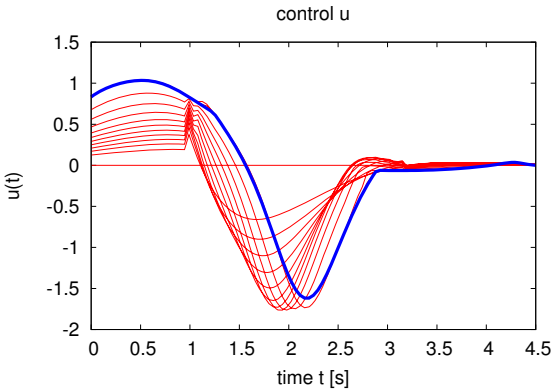
We investigate optimal control problems subject to ordinary differential equations and mixed control-state constraints. Several approaches exist for the numerical solution of such problems. The first approach known as indirect approach is based on the solution of first order necessary optimality conditions which are stated in terms of a minimum principle. A second approach known as direct approach or first-discretize-then-optimize-approach is based on the discretization of the infinite dimensional problem and the solution of the resulting finite dimensional programming problem by suitable programming methods. A third approach known as first-optimize-then-discretize-approach considers the optimal control problem as an infinite programming problem in a suitable Banach space and applies appropriate optimization algorithms like SQP or Lagrange-Newton directly to the infinite dimensional problem.
We will investigate a fourth method which combines the first and the third approach in some sense. The method tries to solve the first order necessary optimality conditions iteratively. Therefore, the necessary conditions are transformed into an equivalent nonlinear but nonsmooth equation

$$F(z) = 0$$

in appropriate Banach spaces using the Fischer-Burmeister function, cf. Fischer [1]. This nonsmooth equation is solved by a nonsmooth Newton's method

$$V_k(d^k) = -F(z^k), \qquad z^{k+1} = z^k + d^k, \qquad k = 0, 1, 2, \ldots,$$

cf., e.g., Qi [2]. The operator V_k is chosen as an element from a suitably defined generalized Jacobian, cf. Ulbrich [3]. We will show the local quadratic convergence under certain regularity conditions and suggest a globalization strategy based on the minimization of the squared residual norm. A numerical example for the Rayleigh problem concludes the article and it is demonstrated that the nonsmooth Newton's method performs very well. The picture shows the iterations of the globalized nonsmooth Newton's method.



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Simulation and Optimal Control of Molten Carbonate Fuel Cells

K. Chudej, K. Sternberg, H.J. Pesch, Univ. Bayreuth, Germany

Corresponding Author: K. Chudej
Universität Bayreuth, Lehrstuhl für Ingenieurmathematik
Universitätsstr. 30, 95440 Bayreuth, Germany
e-mail: kurt.chudej@uni-bayreuth.de

Molten carbonate fuel cells (MCFC) are especially well suited for stationary power plants if their process heat is used to increase their efficiency. MCFCs seem to become soon competitive compared with traditional power plants. The dynamic behaviour of MCFCs can be modelled mathematically by a hierarchy of systems of partial differential algebraic equations in 1D or 2D. Integral terms appear and the nonlinear boundary conditions are given partly by a DAE system.

These large PDAE systems of dimension between roughly 10 and 30 equations are discretized by the method of lines, yielding huge dimensional DAEs.

We will present new numerical results of the optimisation during load changes for a 2D dynamical model including a detailed modelling of the pores. Some comments on time and perturbation indices of these nonlinear PDAEs of mixed parabolic and hyperbolic type will conclude the talk.

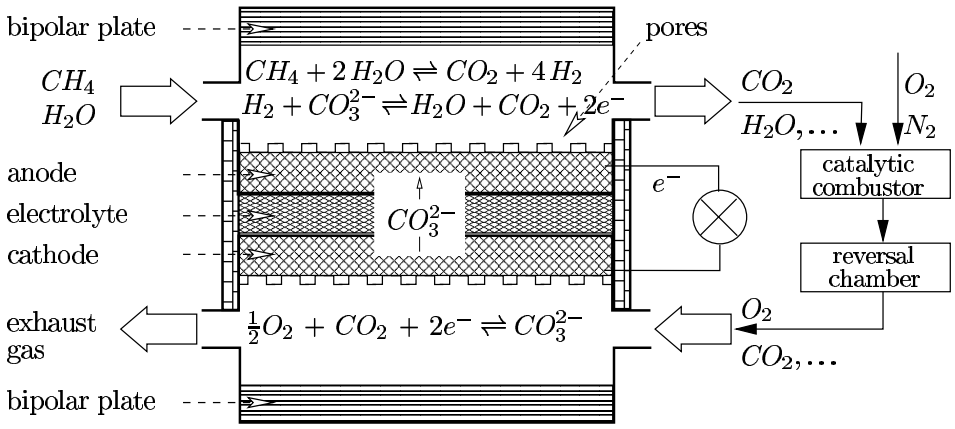

Figure 1: Gas flow and chemical reactions of 1D model

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Optimal Control of Self-Organized Dynamics in Cellular Signal Transduction

D. Lebiedz, S. Sager, O. S. Shaik, O. Slaby, IWR Heidelberg, Germany

Corresponding Author: D. Lebiedz
Interdisciplinary Center for Scientific Computing, University of Heidelberg
Im Neuenheimer Feld 368, 69120 Heidelberg, Germany
e-mail: lebiedz@iwr.uni-heidelberg.de

Recently, increasing experimental evidence has become available supporting the significance of self-organization and pattern formation for information processing in cellular signal transduction [4]. The underlying complex mechanisms can only be understood by help of detailed mathematical modeling, simulation and analysis. In that context, model based control studies of self-organized dynamics are promising for two major reasons. First, to study potential dynamic regulatory mechanisms used by the cell to coordinate its signal transduction activities, and second, to explore possibilities for specific manipulation of biochemical system dynamics by external stimuli and targeted modifications [2] realized for example by tailored drug application and treatment strategies. Optimal control allows the general formulation of inverse problems with time-varying input parameters as well as specific control aims in the form of objective functionals to be minimized.

In this contribution we demonstrate how model-based optimal control of self-organized dynamical processes can be used in biochemical modeling. We consider two applications in which self-organized dynamical processes in form of biochemical oscillations are observed and show how optimal control can be exploited to probe possible signaling routes and to specifically manipulate the biological system to obtain a desired behavior. Model-based control approaches in systems biology may have the long-term potential to contribute to the development of efficient drugs and treatment strategies.

The first process we discuss is the oscillation of a biochemical species in neutrophil granulocytes, special immune cells. After presenting a detailed biochemical model, we argue, based on optimal control results, that the oscillator, which plays an important role in the immune functions of the cells [4], may be dynamically regulated by variable Glucose transport over the cell's plasma membrane.

The second process we study is special biological rhythm, the so called circadian clock. This is periodic process of nearly 24 h which is generated by periodic activation and inhibition of transcription of a set of genes and which is adapted to the periodic day-night cycles and the corresponding physiological activity of many organisms. Based on a kinetic model for the fruit fly Drosophila [3], we apply optimal control to specifically manipulate this rhythm by external light stimuli. We present a novel approach [5] based on Bock's direct multiple shooting [1] to obtain desired bang-bang control functions. In particular, we demonstrate annihilation and restoration of the circadian oscillator.

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Numerical Optimal Control of the Wave Equation: Optimal Boundary Control of a String to Rest in Finite Time

M. Gerdts, Universität Hamburg, G. Greif, Technische Universität Darmstadt,
H. J. Pesch, Universität Bayreuth, Germany

Corresponding Author: H. J. Pesch
Universität Bayreuth, Lehrstuhl für Ingenieurmathematik
Universitätsstr. 30, 95440 Bayreuth, Germany
e-mail: hans-josef.pesch@uni-bayreuth.de

Abstract. In many real-life applications of optimal control problems with constraints in form of partial differential equations (PDEs), hyperbolic equations are involved which typically describe transport processes. Because of their nature being able to transport discontinuities of initial or boundary conditions into the domain on which the solution lives or even to develop discontinuities in the presence of smooth data, these problems constitute a severe challenge for both theory and numerics of PDE constrained optimization.

In the present paper, optimal control problems for the well-known wave equation are investigated. The intention is to study the order of the numerical approximations for both the optimal state and the optimal control variables while analytical solutions are known here. The numerical method chosen here is a full discretization method based on appropriate finite differences by which the PDE constrained optimal control problem is transformed into a nonlinear programming problem (NLP). Hence we follow here the approach *first discretize, then optimize*, which allows us to make use not only of powerful methods for the solution of NLPs, but also to compute sensitivity differentials, a necessary tool for real-time control.
Keywords. Optimal control of partial differential equations; optimal control of hyperbolic equations; optimal control of the wave equation; first discretize, then optimize.

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Process Modelling

BOND GRAPH MODELLING OF AN ADSORPTION PROCESS

A. Baaiu, F. Couenne, Y. Le Gorrec, L. Lefèvre and M. Tayakout-Fayolle
LAGEP, UMR 5007 CNRS / Université C. B. Lyon 1, France

Corresponding Author : F. Couenne,
ESCPE-Lyon Bat 308G, 43 Bd du 11 novembre 1918, F-69622 Villeurbanne Cedex, France.
Phone: +33 4 72 43 18 82, Fax: +33 4 72 43 16 82
Email : couenne@lagep.univ-lyon1.fr

Adsorption process are based on the ability of a solid to preferentially adsorb some molecules present in a fluid phase in order to separate them. The aim of this paper is to present a port-based distributed parameter model of an adsorption column under isothermal conditions using the bond graph terminology.

Firstly, we recall the principles of adsorption process and why it is a spatial multi scale process. We specify the geometry of the considered case and the hypothesis made for the development of our model.

Secondly, the Maxwell-Stefan model [2] is chosen for the molecular diffusion in both microporous and macroporous scales. For the extragranular scale, an axial dispersion model is used. The constitutive laws giving the molar flux with respect to the effort, the gradient of chemical potentials, characterize the resistive elements of the bond graph model.

Thirdly, we provide for each scale the classical mass balance equations as well as the boundary conditions. Moreover we show how the DTF element (it is an interconnection power conserving structure linking the internal variables and the boundary conditions presented in details in a companion paper [1]) permits also to construct the molar density flux due to the diffusion. The port variables of the storage element C are the molar density flow and the molar chemical potential. The second constitutive relation of the C elements are then given: the thermodynamical properties of the mixture give rise to the expressions of the chemical potentials in function of the molar densities.

We also present the coupling between the different scales. These couplings express that there are a continuity of molar flow per unit of volume and the equality of effort at the mutual frontier of the two scales under consideration. Finally, we propose the bond graph model of the entire system and simulation results are presented.

This model can be easily reused as a submodel for modelling purposes. The port variables are clearly identified. Under these assumptions we represent the Gibbs energy and not the internal energy. We do not have the conservation of energy for open systems. For this purpose it will be necessary to take into account the thermal domain with the entropy balance. This will be the next step of this study.

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EFFECT OF NON-IDEAL MIXING ON CONTROL OF COOLED BATCH REACTORS

F. Caccavale, M. Iamarino, F. Pierri, G. Satriano and V. Tufano
Università degli Studi della Basilicata, Potenza, Italy

Corresponding Author: M. Iamarino
Università degli Studi della Basilicata
Via dell'Ateneo Lucano 10, 85100 Potenza, Italy
Phone: +39 0971205208, Fax: + 39 0971205160
email: iamarino@unibas.it

Industrial stirred tank reactors are often characterized by non-uniformities of concentrations and temperature as a result of a non-perfect fluid mixing. Such gradients may strongly compromise the possibility of an accurate reactor temperature control, since non-idealities are often not taken into account by control laws. So, even if satisfactory performance can be locally achieved by the controller, some reactor zones may experience conditions that significantly differ from those monitored. This partial deviation from the desired operative conditions may be responsible for low product quality and, in case of highly exothermic reactions, even for reactor run-away.

In this paper, a compartment model, [1], is proposed to describe the non-ideal mixing in a cooled batch reactor. The model is obtained by subdividing the reactor into perfectly mixed interacting zones and allows to quantify the quality of mixing in terms of a dimensional internal circulation flow rate X_c. A controller-observer control scheme, [2], based on the assumption of perfect reactor mixing, is adopted to control the temperature of the reactor. The observer is used to estimate the reactant concentration on the basis of temperature measurements. This value is then used by a two-loop control law: a first control loop tracks a desired reference for the jacket temperature, while an outer control loop tracks the desired reactor temperature profile.

The performance of the control scheme has been tested in a wide range of fluid dynamics conditions, obtained by varying the value of X_c. Temperature differences inside the reactor increase when X_c decrease due to the less effective mixing; however, negligible temperature error generally affects the compartment whose temperature measurement is chosen as input value for the control scheme. By further decreasing X_c, a critical value is encountered at which the high segregation degree between the compartments leads to reactor run-away. Figure 1.a reports an overall mean temperature error as a function of X_c for two different locations of the temperature sensor, i.e. in a central and in a peripheral reactor region. The first one is affected by a certain delay with respect to the control action; since such a delay increases by worsening the mixing, the mean tracking error increases by decreasing X_c. Moreover, in this case the peripheral compartments strictly remain below the set-point temperature, thus lowering the desired reactant conversion (Figure 1.b) but run-away conditions only arise at very low X_c values. When temperature control input originates from a compartment bordering the jacket, the central region experiences higher temperatures: conversion degree is higher than in the previous case at every X_c, but run-away conditions may appear even at relatively large X_c. For the set of parameters adopted in this work, the critical values of X_c at which run-away conditions onset in the two cases discussed above differ by a factor of 3.

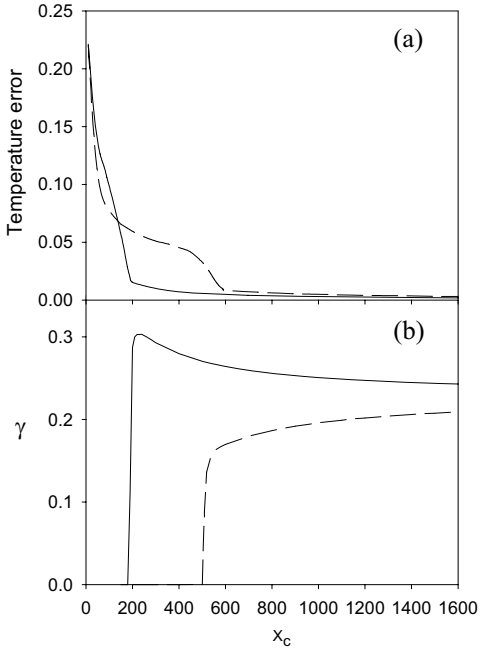

Figure 1. Overall mean tracking error (a) and final dimensionless reactant concentration (b) vs. X_c; temperature sensor location is in a central (solid) and in a peripheral (dashed) reactor region.

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MODELLING OF TEMPERATURE CONDITIONS IN STERILISATION TUNNEL

A. Knoll, M. Atanasijević-Kunc*, R. Karba*

Corresponding Author: M. Atanasijević-Kunc
Krka, d.d. Pharmaceutical Company, Šmarješka cesta 6, 8501 Novo mesto, Slovenia
*Faculty for Electrical Engineering, University of Ljubljana,
Tržaška 25,1000 Ljubljana, Slovenia
Phone: (386) 01-4768 314 Fax: (386) 01-4264 631
email: maja.atanasijevic@fe.uni-lj.si

Large volume parenterals (LVP) are drugs, administered directly into the blood stream of the patient and therefore they bypass most of body's natural defences against infections. It is therefore of vital importance, that the administered drug is sterile. The pharmaceutical production of LVP starts with sterile bottles to fill the product. For sterilisation and depyrogenation of glass bottles or ampoules the so-called sterilisation tunnels are used in pharmaceutical production. These tunnels are usually part of filling lines, where bottles are washed, sterilised filled with the product and finally closed.

During reconstruction of a part of sterile production facilities in Krka, d.d. we installed a new line for production of LVPs. Part of this line is also a tunnel, used for sterilization of glass bottles of different volumes. During the start-up of the line, a set of parameters was recorded for each bottle format, with which the production can run. Due to pharmaceutical production specifications, the operation conditions were far from optimal. Therefore we decided to build a model of temperature conditions of the process. It should enable simulation of temperature profile of each bottle as it travels through the heating zone. With such a model the optimisation of production parameters would be enabled

The bottles are heated up by a stream of laminar air flow that is coming from above and flows through the bottles on the transport belt and by array of infra-red heaters, located below the transport belt. We have decided to divide the model in two parts. The first sub-model corresponds to the bottle, travelling somewhere in the middle of the transport belt and the second to the bottle travelling by its edge.

The start-up measurement of the tunnel's performance resulted in a set of data for each of the six different bottle formats used in our production. Although the temperature profiles seem to be of first order, the sterilisation tunnel proved to be much more complex system. The measurements of temperature profiles on different bottles proved, that first order dynamics will not be sufficient to simulate the behaviour of sterilisation tunnel.

Data sets measured during start-up of the tunnel were used for optimisation of five model parameters. Starting values were either defined on the basis of physical properties tables or deducted from the model behaviour. Model responses are in comparison with measurement data illustrated in Fig.1. The measured values are marked with "*" and simulated values are represented by un-marked lines.

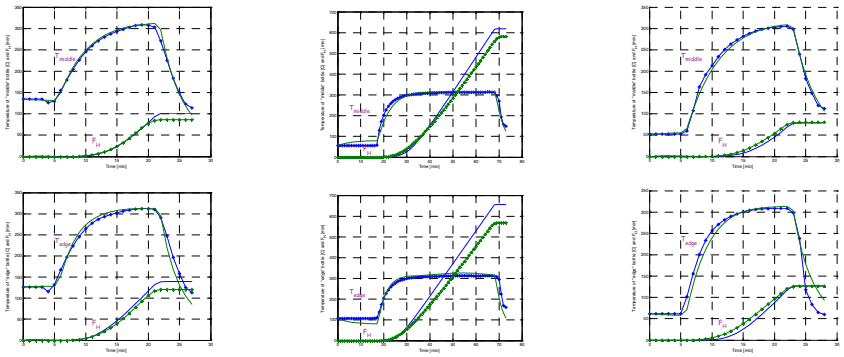

Fig.1: Temperature profiles of three diferent bottles, going through sterilisation tunnel

After several improvements of the model structure and optimisation of several model's parameters we used the model to simulate the situation of malfunctions and we also used the model to optimize some of tunnels production parameters.

Since during production almost no tests on the actual system are allowed, optimisation and forecasting of system's behaviour during malfunctions with help of modelling and simulation has proved to be very efficient.

A MATHEMATICAL MODEL FOR DETECTION OF A PARTIAL BLOCKAGE IN PIPELINES USING FLUID TRANSIENTS

M.S. Ghidaoui, Hong Kong University of Science and Technology,
Hong Kong, China
A.A. Kolyshkin and I. Volodko, Riga Technical University, Latvia

Corresponding author: A.A. Kolyshkin,
Riga Technical University
1 Meza street, block 4, rm. 135, LV 1048, Riga, Latvia
Phone: +371 708 9528, Fax: +371 708 9593
e-mail: akoliskins@rbs.lv

A partial blockage in a pipeline is a common problem in water supply systems and chemical industry. The blockage occurs, for example, when a localized chemical or physical deposition is present at a particular location in the pipeline. Detection and location of the blockage is important in applications since it affects the operation efficiency of the pipeline system. Several methods for blockage detection ([1] – [3]) have been suggested in the literature. The main idea of the method proposed in [3] is the representation of the damping rates for different harmonic components as a sum of the steady-state friction damping factor (R) and the blockage-induced damping factor (R_{nB}). Introducing a small transient in a pipeline, using a time series of pressure measurements and performing a discrete Fourier transform on the time series data one can obtain the sum, $R + R_{nB}$, for each Fourier component $(n = 1,2,3,...)$. The blockage-induced damping factor is obtained by subtracting R from $R + R_{nB}$. It is suggested in [3] that the ratios of the blockage-induced damping rates, R_{nB} / R_{mB}, can be used to determine the location of the blockage and the blockage magnitude.

The solution to the linearized governing equations for a slightly perturbed unsteady flow in a pipeline is obtained in the present paper in the form of the Fourier cosine series with respect to the longitudinal coordinate. The coefficients of the series depend on time and satisfy a coupled system of ordinary differential equations. The system was assumed to be uncoupled in [3] where the solution is found under this (implicit) assumption. It is not a priori clear why such an assumption can be made. Hence, in the present paper the full solution is obtained and the limitations of the mathematical model are discussed in detail.

The analytical solution derived in this paper is based on the traditional one-dimensional waterhammer model, in which the shear stress is approximated by the Darcy-Weisbach steady-state dissipation formulas. The unsteady component of wall shear becomes important when the transient is rapid, the relaxation time of the unsteady wall shear is much longer than the wave travel time, and the application at hand requires that the simulation be conducted over many wave cycles. Nixon et al. [4] tested the damping rate method by applying it to leak-detection problems where unsteady friction is important and concluded that the damping method is valid as long as the computer model used to determine the head trace for the leak-free system can accurately represent the true damping in the pipe under investigation. Similarly, it is expected that the blockage detection formula derived in this paper is applicable provided that the computer model used to determine the head trace for the blockage-free system can accurately represent the true damping in the pipe under study.

It is shown in the present paper that the formula for blockage detection suggested in [3] is valid only in the case where the parameter G (representing the blockage resistance parameter) is small enough. The analysis shows that the formula proposed in [3] represents the leading order term of the asymptotic expansion of the solution in terms of the small parameter G. Thus, the good agreement of the proposed formula with experiments reported in [3] is explained by the smallness of the parameter G.

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RELIABILITY-BASED DESIGN OF INTERMEDIATE STORAGES UNDER GENERAL STOCHASTIC OPERATIONAL CONDITIONS

É. Orbán-Mihálykó, B.G. Lakatos and Cs. Mihálykó, University of Veszprém, Hungary

Corresponding Author: É. Orbán-Mihálykó
University of Veszprém, H-8200 Veszprém, Egyetem u. 10. Hungary
Phone: +38 88 62 42 27, Fax: + 36 88 62 45 21
e-mail: orbane@almos.vein.hu

The intermediate storage plays important role in improving the operating efficiency of processing systems, and fitting to each other the subsystems with different operational characteristics. It increases the availability and variability of systems and reduces the process uncertainties. Most of the works dealing with sizing the intermediate storages for stochastic operation conditions considered batch and/or semi-continuous systems [1, 2]. Orbán-Mihálykó and Lakatos [3] developed a method for reliability-based design of intermediate storages for connecting batch and continuous subsystems when the occurrence times of inputs were governed by Poisson process. The present paper addresses a generalization of this method for the case when both the intervals between the occurrence times of inputs and the amounts of the material transferred by the batch units are described by independent, generally distributed random variables.

The processing system consists of batch and continuous subsystems which are connected by an intermediate storage where the batch units form the inputs of the storage while at the output the material processed is removed continuously with constant volumetric rate into the continuous subsystem. Then the design problem is: specifying the reliability level and the operation period the size of the storage required not to overflow, and the initial amount of material required not to underflow during the operation interval have to be determined.

Integral equations have been derived for the functions $R_1(z,T)$ and $R_2(z,T)$ describing the probabilities of the events of no overflow and no underflow of the storage the solutions to which provide the required designs. Namely, knowing functions $R_1(z, T)$ and $R_2(z,T)$ for a fixed operation interval $[0,T]$ the required initial amount of material in the storage for a given reliability 1-α is determined as $z_0 = R_2^{-1}(1-\alpha)$, while the required volume for no overflow in the storage with reliability 1-α is given as $z_1 = R_1^{-1}(1-\alpha)$. Hence, the required total volume of the storage is $z_2=z_0+z_1$ with the resultant reliability 1-2α.

The integral equations, analyzing the analytical properties of functions R_1 and R_2, were solved by applying stochastic simulation and fitting hyperbolic tangent distribution functions [4] to the simulated data. This method is, in principle, a combination of numerical and analytical methods in which the analytical properties were used in the solution as a priori knowledge. Some results are presented in Fig.1 for a set of parameters where μ and σ with indices F and G stand for the expectation and variance of distributions F and G, describing the distribution functions the time interval between the occurrence times and the sizes of inputs, respectively. The constant removal rate is denoted by c, the operation time is T, storage size and the initial amount of material is z.

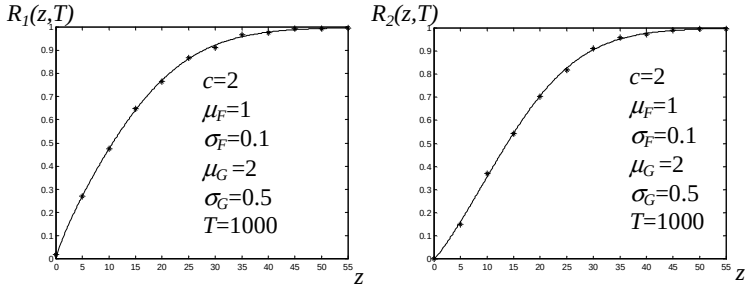

Fig.1. Results of fitting the hyperbolic tangent distribution function to the data obtained by stochastic simulation for probabilities R_1 and R_2

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BLACK-BOX AND FIRST-PRINCIPLE MODEL BASED OPTIMIZATION OF OPERATING TECHNOLOGIES

F.P. Pach, B. Balasko, S. Nemeth, P. Arva and J. Abonyi

Corresponding Author: J. Abonyi,
University of Veszprem
P.O. Box 158. H-8201 Veszprem, Hungary
Phone: +36 88 624-209, Fax: +36 88/624171
email: abonyij@fmt.vein.hu

In modern chemical process systems the technological databases (created by automatic data logging) provide potentially usufel sources of insight for engineers and supervisors to identify causes of poor performance and opportunities for improvement. Such sources store huge amount of data from the production, but they have not been adequately exploited. It is estimated that only 5-10% of commercial databases have ever been analysed.

The formulated products (e.g. plastics, polymer composites) are generally produced from many ingredients, and large number of the interactions between the components and the processing conditions all have the effect on the final product quality. Therefore exhaustive process analysis methods of technological data sources is need to be the first task in requirements of an optimization method.

In this paper a new methodology for optimization of operating technologies is presented, especially how black-box and first-principle models are used together to process analysis. The analysed production process is the PolyPropylene-4 plant (PP4) of TVK Ltd. (www.tvk.hu).

In industrial technologies the being of the distributed control system (DCS) is a basic requirement. This system assures on local the secure and safety operating of the technology. Moreover on the coordinating level there are many alternatives to use the models with different information content to tuning the regulations, optimization, the model identification and the error diagnostic. Because these solutions based on measured data which are originated from the operating, the most DCS have functions to data storing. These data are limited accessible in time on the process control computers, they are archived retrospective about 1-2 months. If we want to store technology data more length of time interval, it is expedient to store data in a database, or special in a process data warehouse. A process data warehouse is a data analysis-decision support and information process unit, which is operated separately from the databases of the DCS. It is an information environment in contrast the data transfer-oriented environment, which contains trusted, processed and collected data in order to historic analyzes, so it makes possible to get relevant information from the technology.

Therefore first step of our method is collect all available data and technology information into a process data warehouse. The process flow diagrams of the production process are more informative by drawing the codes of process controllers taken from the P&I-s and by detecting the main control circles. Then the process control model of the APC (Advanced Process Control) controller is implemented in Matlab® Simulink® environment to analyze the sensibility of products to the process values, to achieve product lifetime analysis and to be able to work out brand new bias points for product circles in the future period. The model uses the process data warehouse as data source.

To analyze the enormous amount of data (stored in process DW), statistical data analysis tools are needed: trend diagrams, box plots, quantile-quantile plots, etc. Data mining tools as association rule mining, classification and clustering algorithms are also can be applied to get relevant information about the technology. The statistical analysis and data mining tools are also implemented in Matlab®.

The main goal of our process analysis methodology is to discover as many relevant features and relationships of the production process as possible based on the proposed tools. Based on the application of the proposed tools and the analysis of the results, several rules have been extracted. Most of these rules found to be useful for our industrial partner, since the extracted knowledge and the resulted plots can be effectively used to summarise trends of the process variables and estimate the quality of the products. The behaviour of the control algorithm of the advanced model-based control system can be also identified from these analysis.

DYNAMIC MODELLING OF A pH NEUTRALIZATION PLANT FOR CONTROL

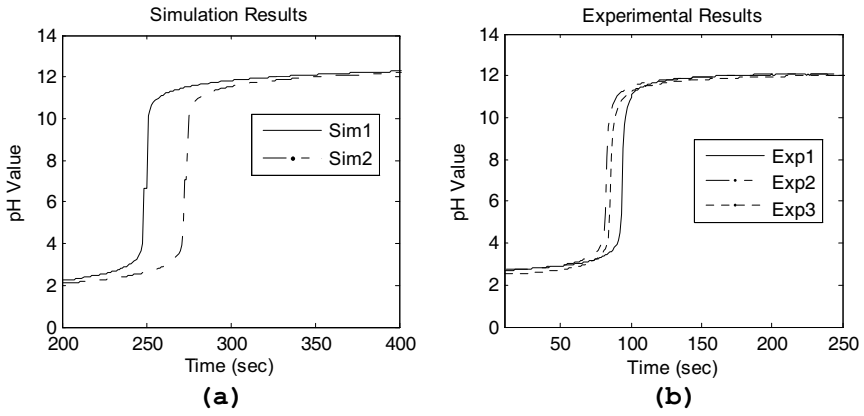
Rosdiazli Ibrahim[1] and David J. Murray-Smith [2]

Department of Electronics and Electrical Engineering
Rankine Building, Oakfield Avenue
Glasgow, G12 8LT, United Kingdom
Phone: +44 0141 330 8631, Fax: + 44 0141 330 4907
email: ribrahim@elec.gla.ac.uk[1] and D.Murray-Smith@elec.gla.ac.uk[2]

The control of a pH neutralization plant presents a challenge due to the time-varying and nonlinear dynamic characteristics of the process. This paper discusses the groundwork for the development of a mathematical model of a pilot plant derived from physical and chemical knowledge. Although modelling of a pH neutralization process is not a recent issue, as mentioned at the beginning of the paragraph, the behaviour of this reaction process is complex and highly nonlinear.

The eventual aim in developing the pH neutralisation process model is to design and implement a control scheme. The model will thus be used to develop a control strategy for the system using nonlinear model-based predictive control (MPC) methods. Such a control strategy depends upon predictions based on the nonlinear model of the process and the overall performance of the controlled system depends, therefore, upon the quality of the process model

Sets of experimental data from the pilot plant have been used for the external validation of the mathematical model and the associated computer simulation. The pilot plant uses industrial instrumentation and measurement technology. It is therefore representative of an actual pH neutralization plant used in industry. The paper focuses on an investigation of the reliability and accuracy of the mathematical model obtained from a physico-chemical approach compared with the actual pilot plant characteristics. Therefore, the comparison and evaluations of the performance of the mathematical model compared with the plant behaviour is an important feature of this paper. As an example two titration curves are shown below: (a) simulated results for two sets of conditions using the developed mathematical model, (b) an experimental result obtained from three separate tests on the pilot plant. Analysis of the results suggests that the mathematical model can describe the experimental curves to a level of accuracy that is adequate for the control application. From this, and other evidence, it is believed that the development of the nonlinear dynamic model for the pH plant has been successfully achieved.



This research involves collaboration between the University of Glasgow, UK and the Universiti Teknologi Petronas (UTP), Malaysia. The pilot plant (pH neutralization plant) is available at the Plant Process Control Laboratory, in UTP. The authors wish to thank both parties for their support and assistance.

MODELLING AND OPTIMIZATION OF HIERARCHICAL STRUCTURES

Tiit Riismaa

Institute of Cybernetics at Tallinn University of Technology
Akadeemia tee 21, 12618 Tallinn, Estonia
Phone: +37 2 6204192, Fax: +37 2 6204151
email: tiitr@ioc.ee

Consider all *s*-levels hierarchies, where nodes on level *i* are selected from the given disjoint sets and all selected nodes are connected with the selected nodes of adjacent levels. Suppose $Y_i (i = 1,...,s)$ is the $m_i \times m_{i-1}$ adjacent matrix of levels *i* and *i*-1, $m_s = 1$. All hierarchies from the set described above satisfy the condition $Y_s \cdot ... \cdot Y_1 = (\underbrace{1,...,1}_{m_0})$.

Consider the general hierarchy optimization problem:

$$\min \left\{ \sum_{i=1}^{s} \sum_{j=1}^{m_i} \mathrm{h}_{ij} \left(\sum_{r=1}^{m_{i-1}} d^{\,i}_{jr} y^{\,i}_{jr} \right) \middle| Y_s \cdot ... \cdot Y_1 = (\underbrace{1,...,1}_{m_0}) \right\} \text{ over } Y_1,...,Y_s. \quad (1)$$

Here $h_{ij}(\cdot)$ is an increasing loss function of *j*-th element on *i*-th level and $d^{\,i}_{jr}$ is the element of $m_i \times m_{i-1}$ dimensional cost matrix D_i for the cost of connection between the *i*-th and (*i*-1)-th level. The argument of function $h_{ij}(\cdot)$ in (1) describes the connections of *j*-th element on level *i*. The first two sum signs correspond to the loss over all levels and over all elements inside of *i*-th level respectively.

A recursive algorithm where index of level is the index of recursion is constructed to solve the problem (1).

Consider a special case where the connection cost between the adjacent levels is the property of supreme level. Suppose additionally that $h_{i1}(k) \le ... \le h_{im_i}(k) (i = 1,...,s)$. Now the optimization procedure (1) falls into outer and inner mutually dependent phases:

$$\min \left\{ \sum_{i=1}^{s} g_i (p_{i-1}, p_i) \middle| (p_1,..., p_{s-1},1) \in W^s \right\} \text{ over } p_1,..., p_{s-1}, \quad (2)$$

$$g_i (p_{i-1}, p_i) = \min \left\{ \sum_{j=1}^{p_i} h_{ij}(k_{ij}) \middle| \sum_{j=1}^{p_i} k_{ij} = p_{i-1} \right\} \text{over} k_{i1},...,k_{ip_i}; W^s = \left\{ (p_1,..., p_{s-1},1) \middle| 1 \le p_i \le p_{i-1} \right\}. \quad (3)$$

Here variable parameter $p_i (i = 1,...,s-1)$ is the number of nodes on level *i* (p_0 is fixed, $p_s = 1$) and variable parameter $k_{ij} (i = 1,...,s;\ j = 1,...,m_i)$ is the number of edges outgoing from the *j*-th node on level *i*.

If functions $h_{ij}(\cdot) (i = 1,...,s)$ are discrete-convex [1, 2], then objective function of problem (2) – (3) is discrete-convex [2]. A recursive algorithm where index of level is the index of recursion is constructed to solve the problem (2) – (3). Also a numerical method of local searching is developed. On each step of the iteration the calculation of the value of objective function is required only on some vertices of *s*-dimensional unit cube.

The considered approach is illustrated by optimization of the structure of multi-level processing system.

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MODELLING AND FEEDBACK CONTROL OF THE STARTUP PROCESS OF EMPTY COLD REACTIVE DISTILLATION COLUMNS: THE FILLUP AND HEATING CASE

S. Sommer, J. Raisch and K. Sundmacher, Max Planck Institute Magdeburg, Germany

Corresponding Author: S. Sommer
Max Planck Institute Dynamics of Complex Technical Systems
Sandtorstr. 1, 39106 Magdeburg, Germany
Phone: +49 391 6110-379, Fax: + 49 391 6110-399
email: stsommer@mpi-magdeburg.mpg.de

Reactive distillation (RD) processes integrate chemical reactions and distillation in the same process unit [3]. This has several positive implications, for instance reduction of investment and operational costs and potential improvement of performance. However, the dynamic behavior of reactive distillation columns (RDC) is quite complex, especially during the startup stage.
The startup process of RDC is of environmental and commercial importance, and represents an active field of research. For RD operation, startup should be finished as fast as possible since all process variables are changing during this stage, and the product has to be disposed. For this purpose, suitable control strategies are needed. So far, there are only few publications addressing startup of empty cold RDC, for instance [1,2].

The motivation of this paper is to solve the problem of the complete startup process of the cold empty column by means of feedback control strategies, which is not reported so far in the literature. The use of feedback implies several potential advantages when compared to the existing open loop strategies: for example the startup process can be made insensitive against disturbances, operating safety can be improved, and a desired steady state can be reached exactly.

It is convenient to model different stages of the startup procedure separately and to apply a different control strategy for each stage. The outcome is a switching scheme consisting of several control policies based on different models.

In this contribution, we investigate the first stage of startup. Here, the aim is to fill the lower part of the column (below the feed location) and to heat the reboiler to obtain boiling conditions within a given time interval. This stage is relevant, because in most works on startup of RDC the trays are filled and warm.
A rigorous model is developed to describe the first part of startup. For each tray, one total mass balance, one energy balance, and nc-1 component mass balances are formulated (nc = number of components). The generated equations are a rather complex, nonlinear, and implicit differential algebraic equation (DAE) system.
We demonstrate that a simple control scheme consisting of two single PI control loops including anti-reset windup is adequate. In particular, we propose to use the feed flowrate to control the reboiler liquid holdup, and the reboiler heat duty to manipulate the reboiler temperature. The bottom flowrate is set to its desired steady state value. This control strategy is combined with recycling partial bottom product back to the feed (bottom product recycling). This approach features a number of advantages, e.g. the recycle can reduce the amount of waste during startup, and the trays above the reboiler are heated before being reached by vapor.

Our startup strategy has been tested for an example where ethyl acetate and water is produced from ethanol and acetic acid. Promising simulation results have been obtained. The approach with bottom product recycling is recommended for the presented fillup and heating stage.

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Economic Systems

Modelling Advertising Effects - A Hybrid Approach using ODEs and Cellular Automata

Jürgen Wöckl*, Daniel Leitner†

In this paper we describe a simulation approach to explore different advertising strategies in a heterogeneous consumer market. The main focus is to model the dynamic of two competing advertising channels and their dynamic advertising effects. Here one advertising channel effects all consumers at the same time representing traditional large-aera advertising intruments as broadcasting or print media, and the second represents the circulation of post-purchase information in the personal environment of the consumer - called word-of-mouth advertising.

Therefore a model of an artificial consumer market (Buchta/Mazanec 2001, Schuster/Wöckl 2005) has been used to provide an experimental environment for the simulation and optimization task. The ACM provides several factors of interest to make sure all focused marketing and management related strategies can be considered. Optimization methods are applied to the artificial market to derive optimal strategies obtaining maximal profits to keep competitive.

Structually the artificial consumer market is made up of a constant number of consumers represented by the cells of a cellular automata. The position of the cells in the population lattice of the cellular automata represents a local position of the consumer. Additionally to the local position each consumer has a set of internal states. Especially each consumer has an individual aspiration point of attributes which the preferred product should possess. In this study three equal sized segments are assumed each representing a group of consumers with similar aspiration points and three products are established in the market competing for a market share in this artificial market. In this environment it's assumed that each firm just provides one product and therefore the profit of the firm equals the price times sales of its product reduced by the budget spent for advertising.

The design of the cellular automata environment is done object-oriented and has been implemented in Java. The lattice has a dimension of 50x50 cells and a bicubic interpolation has been used to produce a smooth graphical representation. The update rule of the CA describes the information flow between consumers sharing their post-purchase satisfaction. At each discrete update-periode of the CA each consumer chooses the best-fitting product, which enables a correction of his pre-purchase attitude by comparing it with the perceived real attributes/features. The firms' target is to optimize their profit, especially the strategic decision between promoting real features or using claims optimized to the segments.

*Institute for Production Management, WU-Wien; juergen.woeckl@wu-wien.ac.at
†ARGESIM, TU Wien; dleitner@osiris.tuwien.ac.at

THE PRINCIPLE OF PARSIMONIOUS MODELLING IN ECONOMIC GROWTH EMPIRICS - COMPARING DATA-DRIVEN APPROACHES

B. Brandl, Ch. Keber and M. Schuster, University of Vienna, Austria

Corresponding Author: B. Brandl
University of Vienna
Brünner Straße 72, 1210 Vienna, Austria
Phone: + 43 1 4277 - 38314, Fax: + 43 1 4277-38318
email: bernd.brandl@univie.ac.at

The aim of this paper is to investigate data-driven approaches in automated modelling in the light of the principle of parsimonious modelling. The question of what variables should be considered in modelling is now a challenge as a large number of candidate variables are available but not all can be included. Even in cases where more observations than variables are available, concerns for the precision of estimates will necessitate restricted models. The principle of preferring smaller models whenever they yield the same descriptive accuracy as larger ones is usually labelled as the principle of parsimoniously but also called 'Occam's razor'. This problem is observable in all fields of empirical economics but the most prominent debate is held in economic growth empirics. Since [3] in empirical economic literature data-driven approaches in modelling became increasingly necessary and popular as the number of explanatory variables increases rapidly. Traditional econometric modelling has problems in dealing with this phenomenon so that data-driven approaches are needed. We exemplify our investigation by joining the debate on empirical economic growth modelling which literature in this field has triggered in the last few years. We will show that one major disadvantage of frequently applied data-driven approaches is that they do not consider the principle of parsimonious modelling, which is, as we will argue, a disadvantage as these results are either too parsimonious in the sense that their explanation is limited or they are too rich in the sense that statistical adequacy suffers. In contrast to other data driven modelling approaches we suggest applying a judicious selection of subset of models using a genetic algorithm for finding an optimal solution which takes into account the principle of parsimonious modelling. At present the use of a genetic algorithm as a method for automated, data-driven modelling is promising since genetic algorithms have rarely been applied in the recent debate on algorithms for analysing causal structure among variables. We compare the other approaches in their ability to model a parsimonious solution by defining the quality of the parsimonious modelling results by well-known measures like the Akaike information criterion, the Hannan-Quinn information criterion and the Bayesian information criterion. Our results showed that the use of a genetic algorithm performed efficient stochastic exploration of the search space with a population of models that progressively adapt to the given data and automatically find the dependencies among explanatory variables and, thus, they identify which variables should enter the model under principles of parsimonious modelling. Using the same data as [1] and [2] - which is also similar to the data in [3] - we achieve different results when compared to applying other data driven approaches such as the extreme bounds test and the general-to-specific approach. In context of empirical determinants of economic growth we were able to show that specifications that are guided by the principle of parsimonious modelling see more variables worth being considered compared to previous findings in literature.

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A Nonlinear Analytical Dynamic Model for the Iranian Male Labour Supply

A. Aghaei, H. Shakouri G., Tehran University, and M. Karrari, AUT, Tehran, Iran

Corresponding Author: A. Aghaei
Amirkabir University of Technology
Hafez Ave, Tehran, Iran
Phone: + 98 21 6646-6009, Fax: + 98 21 6640-6469
email: a_aghaei_57@yahoo.com

Abstract. One of the most important problems in macro-economics, is the unemployment rate prediction. The unemployment rate is caused by labour market performance, which consists of two parts: the labour supply and the labour demand. Interactions of these two parts determine the unemployment rate. In order to influence the market behaviour, it is necessary to model both parts for both male and female labour supply. Most of the labour forces in Iran are male. Rapidly growing population in the two past decades plus the weakness of economy growth resulted in high rate of unemployment. In this paper, an analytical dynamic model is developed for the Iranian male labour supply. The lifecycle theory is used to divide the male labour supply into three age groups:

1. Age group of 10 to 19 years: The most of people usually have a primary education.
2. Age group of 20 to 24 years: Some people usually have an undergraduate education.
3. Age group of 25+: Some people often have a graduate education or higher.

All models for different male labour supply groups have the common. This structure considers the influence of economical and demographical variables into the rate of changes in labour supply population, based on the system dynamics approach.
Then the static theory is used as a basis to construct each model analytically. Through those models, it has been presented that some criteria such as education level, marriage and the history of unemployment rate can strongly affect on the labour supply as well as the real wage rate and real non-labour income, which have both the substitution and income effects. Moreover, a reservation wage is estimated for each model.

In this research, the Genetic Algorithm and Direct Search techniques are used to estimate the parameters. A least square method is applied, and various validation criteria, such as the simulation error, prediction error, R2, etc., are calculated. Moreover, the parameters are checked to be significant with the correct expected signs. The Results show a high accuracy in the model: R2 is above 0.995 for all models; the maximum prediction error for the unused samples is less than 0.001, and the t-student statistics of all parameters is more than 1.1. In all models, the unemployment rate and ratio of student per population variables have the negative effect on labor supply. Moreover, as it is expected, the ratio of labor force with high education per the whole population and the ratio of married people per population have the positive effect. It means that both educations and marriage cause the labor supply to increase. As another result, it is seen that if the non-labor income increases the labor supply is decreases. However, the real wage rate has the substitution effect on male labor supply from 10-19 ages and has the substitution and income effects on other age groups.

Keywords. Mathematical Modelling, Dynamic Models, Nonlinear Models, Labour Supply, Labour Market Dynamics

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Control-oriented Modelling of Advanced Multi-Link Manipulators

OBJECT-ORIENTED DYNAMICS MODELING OF WALKING ROBOTS FOR MODEL-BASED TRAJECTORY OPTIMIZATION AND CONTROL

R. Höpler[1], M. Stelzer[2], and O. von Stryk[2]

[1] TESIS DYNAware GmbH
Baierbrunnerstrasse 15, 81379 Munich, Germany
email: robert.hoepler@tesis.de

[2] Technische Universität Darmstadt
Hochschulstrasse 10, 64289 Darmstadt, Germany
Phone: + 49 6151 16-4722, Fax: + 49 6151 16-6648
email: stelzer@sim.tu-darmstadt.de

Modeling of walking robots is an intricate subject when dealing with optimization and model based control. The resulting multibody systems with a free floating base lead to high dimensional equation systems and a frequently changing kinematic structure due to time-varying contact situations. However, specialized algorithms that treat the contacts separately and thus may make use of the tree structure of the system can be applied. This paper discusses the development and application of object-oriented modeling and implementation techniques to achieve a representation of the mechanical model amenable to the various requirements by legged robot applications. This leads to a uniform, modular, and flexible code generation while reaping the performance of efficient domain-specific articulated body algorithms.

Trajectory optimization problems of bipedal and quadrupedal robots are investigated as applications. The optimal control problems involve different optimality criteria such as energy or time and involve the complete dynamics of the system as side conditions as well as several nonlinear inequality and boundary constraints that ensure stable, symmetric gaits. It is shown how a high-level specification of multibody dynamics models using component libraries serves as a basis for generation of a number of modules forming an “overall” computational dynamics model tailored to the needs of the optimal control techniques involved. Exact sensitivities may be calculated directly from the dynamics algorithm and thus in future might help for better convergence of the optimal control problems.

The selected examples illustrate how this approach tackles the emerging complexity by integrating various algorithm modules for, e.g., equations of motion, non-linear boundary conditions, symmetry and transition conditions, for multiple phases that differ in the number of legs in contact with ground during motion. Variations of the mechanical structure, e.g., contact conditions can be treated either by multiple models or by reconfiguration of one model.
Parts of the model may be used, e.g. one single leg for considerations of the leg swing height. Numerical results are presented for time- and energy-optimal walking trajectories of full three-dimensional models of a humanoid robot and a Sony four-legged robot.

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MODELING AND OPTIMAL CONTROL OF MULTIPLE CONSTRAINED MANIPULATOR MOTION ON MANIFOLDS

S. Breun and R. Callies

Munich University of Technology
Boltzmannstr. 3, 85748 Garching, Germany
email: breun@ma.tum.de and callies@ma.tum.de

In a large variety of industrial applications such as assembly lines or welding stations , robotic manipulators are used to an increasing degree. To fully exploit the capacities of multi-link industrial robots and to achieve high working performance, manipulator tasks have to be carefully optimized. In many applications it is necessary to move the end-effector of a manipulator along a prescribed path in minimum time. Early algorithms for calculating time optimal controls for this class of problems have been developed e.g. by [1]. These algorithms are limited to special classes of problems because structural information of the control is necessary. A similar problem with a mixed time-energy objective function has been investigated by [5], who uses optimal control theory to derive necessary conditions for an optimal solution which is then obtained by solving a boundary value problem. Only control constraints are taken into account; additional assumptions are made to avoid the complicated treatment of state constraints that result from the control constraints after transformation to path coordinates. In industrial applications these optimal control problems are mainly solved by so-called direct methods. These are based on a discretisation of the control variables – and often the state variables too – and do not have to deal with necessary conditions from optimal control theory explicitly. For realizations see e.g. [2], [4], [6].

In this paper, time-optimal trajectories for a three-link robot are investigated subject to path constraints of the type described above. A Maximum Principle based approach is applied taking into account the full set of relevant control and state constraints. Additional state constraints such as bounds on the angular velocities are handled simultaneously. A simpler structure of the problem is achieved by the transformation into minimum coordinates; the price to be paid is the occurence of two highly nonlinear mixed control and state constraints and additional state constraints of first order. In case of touch points of the state constraints with both control constraints being active simultaneously, new interior point conditions are derived. The complete optimal control problem is transferred into a nonlinear multi-point boundary value problem. By the use of the adjoint variables structural properties of the optimal control problem are revealed and a priori estimates of the control structure are replaced by homotopy techniques. The fast numerical solution is by the advanced multiple shooting method *JANUS* [3].

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BILEVEL OPTIMIZATION OF CONTAINER CRANES

C. Büskens and M. Knauer

Universität Bremen
Zentrum für Technomathematik, Fachbereich 03
Postfach 33 04 40, 28334 Bremen, Germany
Phone: +49 421 218-2413, Fax: +49 421 218-4235
email: bueskens@math.uni-bremen.de
email: knauer@math.uni-bremen.de

Infinite dimensional bilevel optimal control problems are presented as an extension of classical bilevel optimal control problems and single-level optimal control problems. Hereby, additional constraints are considered for the primary problem, which depend on the optimal solutions of secondary optimal control problems.

A demanding problem arises with the complexity of the problem, since the primary optimal control problem has to be solved depending on an infinite number of secondary optimal control problems contrariwise depending on the primary problem. The secondary optimal control problems have to be solved for any given point in time of the primary problem. Moreover, primary and secondary problems work on different variables in time.

The numerical solution of the bilevel approach is illustrated by an application of a container crane. Jerk and energy optimal trajectories with free final time are calculated under the terminal condition that the crane system comes to be at rest at a predefined location. In enlargement, additional constraints are investigated to ensure that the crane system can be brought optimally to a rest position at a free but admissible location from any state of the trajectory.

For the optimal solution of the bilevel programming problem for the container crane, Figure 1 shows the velocity $\dot{s}(t)$ of the trolley, the change in the length of the wire rope $\dot{l}(t)$ and the relative velocity $\dot{d}(t)$ of the payload of the crane system with respect to the trolley. The main trajectory is drawn along the axis to the left. Additionally, a collection of 15 associated stop trajectories branch along the axis to the right. For each stop trajectory, these states are actually controlled to zero, as it was requested in the problem formulation.

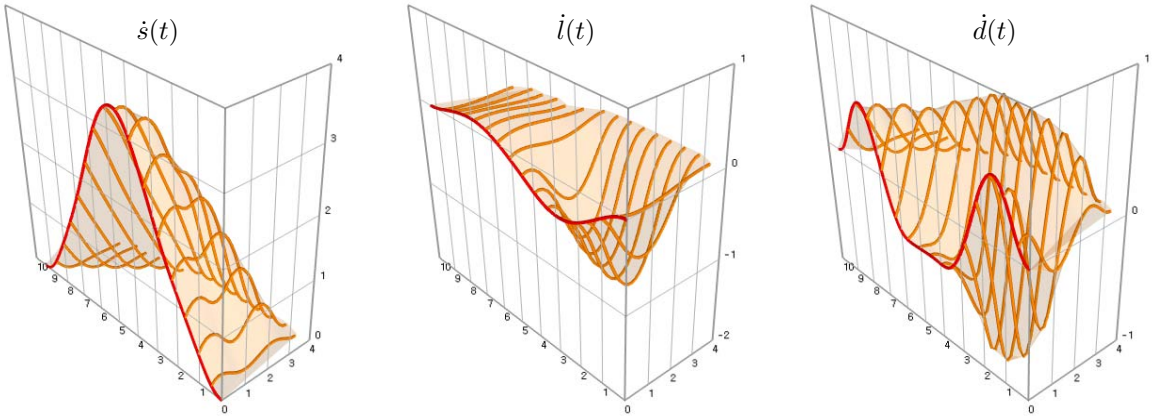

Figure 1: Optimal solution of the main trajectory and its associated stop trajectories.

INTRINSIC MODELING OF MECHANICAL SYSTEMS BASED ON GEOMETRY

M. Schöberl and K. Schlacher,
Johannes Kepler University Linz, Austria

Corresponding Author: M. Schöberl
Institute of Automatic Control and Control Systems Technology
Altenbergerstraße 69, 4040 Linz, Austria
Phone: +43 732 2468 - 9735, Fax: + 43 732 2468 - 9734
email: markus.schoeberl@jku.at

The goal of this contribution is to show how differential geometric concepts appear in the context with mechanics. The fact that bundles are the appropriate object to describe Newtonian mechanics follows from the assumption that each event in space-time has a well defined time. In the language of bundles this means that all events that take place at the same time lie in one and the same fibre over the base manifold which represents the time. To measure the distance between two events in space-time one has to introduce a metric. It is obvious that this metric has to be a vertical metric since one only can measure the distance between events that lie in the same fibre. The definition of the velocity and the acceleration of a mass point is the crucial step to understand point mechanics. It turns out that the introduction of connections is essential for a coordinate invariant definition of the velocity and the acceleration. The concept of a connection directly leads to a first order differential operator, called the covariant differential, which will be used to calculate the change of certain objects along the evolution of a mass point in an intrinsic manner. Since we insist on a description which is invariant with respect to all possible choices of coordinates that preserve the bundle structure this approach consequently also deals with the possibility of accelerated coordinate systems. This leads to a non trivial space-time connection and to the observation that the velocity of a motion is a vertical field on the space-time bundle with respect to the fibration. It is well known, that the Levi-Civita connection is important when describing the acceleration of a mass point in a space which possesses a metric that is not flat. However, the Levi-Civita connection is not the appropriate tool when considering accelerated coordinate systems and therefore it is our intention to exploit the geometry of the space-time bundle in such a way, that it is also possible to take the case of an accelerated coordinate system into account.

The most popular mathematical descriptions for a continuum are the Lagrangian and the Eulerian formulation. It will turn out that the definition of the velocity and the acceleration in this intrinsic manner as discussed for point mechanics can be adopted to the case of a continuum in a straightforward manner. We will present the mass balance and the balance of linear momentum and it has to be emphasized that the main difference between point mechanics and continuum mechanics is the fact that one is confronted with vector valued forms instead of vectors. This observation leads to the introduction of mathematical tools such as the codifferential. As an example we will show how the partial differential equations that appear in the Lagrangian setting can be reduced to describe a rigid body motion.

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RECURSIVE MODELING AND CONTROL OF MULTI-LINK MANIPULATORS WITH VACUUM GRIPPERS

R. Callies* and S. Fronz†
*Munich University of Technology, Germany
†P+Z Engineering GmbH, Germany

Corresponding Author: R. Callies
Centre for Mathematical Sciences M2, Munich University of Technology
Boltzmannstr. 3, 85748 Garching, Germany
email: callies@ma.tum.de

Manipulators equipped with vaccum grippers are a new and flexible element in innovative material-flow solutions. The limited holding forces of vacuum grippers require elaborate strategies of control to prevent the contact between gripper and load from breaking off especially in time optimal motions with high acceleration forces active. Mathematically this can be modeled as a constraint on internal forces of a multi-link manipulator.

The manipulator model reflects the main properties of a typical industrial robot with vacuum grippers. It is based on the rigid body formulation of a manipulator with n rotational joints and an anisotropic model of the vacuum gripper's holding force. The equations of motion have the following fundamental structure

$$\begin{pmatrix} \dot{\Theta}(t) \\ \dot{\Phi}(t) \end{pmatrix} = \begin{pmatrix} \Phi(t) \\ M^{-1}(\Theta(t))\,(T(t) + h(\Theta(t), \Phi(t), t)) \end{pmatrix}$$

Time $t \in [t_0, t_f]$ is the independent variable, the vector of the link angles $\Theta := (\theta_1, \ldots, \theta_n)^T \in \mathbb{R}^n$ denotes the state variables and $\dot{\Theta} = \Phi, \ddot{\Theta} \in \mathbb{R}^n$ the generalized velocities and accelerations. n is the number of joints, $M = M(\Theta) \in \mathbb{R}^{n \times n}$ the mass matrix (in the ideal rigid body case positive definite and symmetric), and $h = h(\Theta, \Phi, t) \in \mathbb{R}^n$ contains e.g. the moments resulting from gravitational, centrifugal and Coriolis forces. The torques $T := (T_1, \ldots, T_n)^T \in \mathbb{R}^n$ are the control variables. They are subject to the additional constraints $T_i(t) \in [T_{i1}(t), T_{i2}(t)]$ with given $T_{i1}(t) \leq T_{i2}(t)$, $i = 1, \ldots, n$, thus including active and passive joints. A seamless inclusion of the gripper and load into the formalism is possible. The gripper is fixed to link $n-1$ and modeled as part of this link; the load of mass m_n is modeled as link n connected to link $n-1$ by the immobile (artificial) joint $n-1$ ($\dot{\theta}_n = 0$, $\ddot{\theta}_n = 0$).

The equations of motion are calculated by the Newton-Euler recursion in an implicit form (inverse dynamics): For every input vector $(\Theta, \dot{\Theta}, \ddot{\Theta})^T$ the recursion delivers

$$T(\Theta, \dot{\Theta}, \ddot{\Theta}) = M(\Theta)\ddot{\Theta} + h(\Theta, \dot{\Theta})$$

The derivatives $\dfrac{\partial T_i}{\partial \theta_j}(\Theta, \dot{\Theta}, \ddot{\Theta})\,, \quad \dfrac{\partial T_i}{\partial \dot{\theta}_j}(\Theta, \dot{\Theta}, \ddot{\Theta})\,, \quad i, j = 1, \ldots, n$, are obtained by differentiating the Newton-Euler recursion with respect to θ_j, $\dot{\theta}_j$. For every joint j, this differentiation process again results in an outward and an inward recursion. Based on this core information, all the information required for a Maximum Principle based approach to the optimal control problem (formulation of the adjoint differential equations, evaluation of the optimality conditions) is easily accessible.

The anisotropic constraint on the vacuum gripper is transformed into two state constraints $C_i(T, \Theta, \Phi) \leq 0$, $i = 1, 2$, of order 0, which are evaluated using internal information from the above recursions and complementing it by another specialized recursion of similar structure.

By these measures, the modeling of the complete optimal control problem and its transformation into a piecewise defined, highly nonlinear multi-point boundary value problem is automated to a great extent; the fast numerical solution of the boundary value problem is by the advanced multiple shooting method *JANUS*.

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Tool Integration and Interchange Formats for Hybrid Systems

TOOL INTEGRATION FOR HYBRID SYSTEMS IN HYCON

Manuel A. Pereira Remelhe, Sebastian Engell

Corresponding Author: Manuel A. Pereira Remelhe
Department of Biochemical- and Chemical Engineering
Universität Dortmund,
44221 Dortmund, Germany
Phone: +49 231 755-5171, Fax: +49 231 755-5129
m.remelhe, s.engell@bci.uni-dortmund.de

Within the European Network of Excellence HYCON different approaches for integrating tools that cope with hybrid systems are being investigated and realized. Hybrid systems exhibit continuous dynamics as well as discrete event dynamics. This article shows the need for model exchange among different tools, explains the difficulties connected to it, and presents some intermediate results and plans for the near future. In contrast to other approaches for tool interoperability that try to solve the related problems in a uniform way, in HYCON, horizontal and vertical integration are distinguished resulting in a package of concerted methods and exchange formats dedicated to specific analysis methods and different levels of abstraction.

In the hybrid systems paradigm a system exhibits interacting continuous and discrete event dynamics. This enables an intuitive representation of technical systems composed of parts governed by the continuous laws of physics and chemistry as well as controllers monitoring the measurements from the physical system and reacting to certain events by discrete actions via the actuators. However, whether a system is considered as a purely continuous, a purely discrete, or a hybrid system is a matter of the chosen level of abstraction and depends strongly on the modeling purpose.

Many methods and tools have been developed for hybrid systems in the last decade that can not be combined directly to solve a complex problem due to the lack of an agreement on a common unifying formal basis and the resulting large number of different modeling languages. Each language has its specific features and semantics that are tailored to a certain application domain or to the analysis methods applied to the models. If an engineer wants to combine different tools in order to exploit their specific functionality or specific expressiveness, he or she has to have profound knowledge on the different formalisms and translate models and results manually which is a very intricate task. This is an unsatisfying situation prevents a broader acceptance of hybrid systems tools.

The ultimate goal in HYCON is to provide a platform supporting several tools that can be seamlessly integrated to solve a particular control design problem. Such a platform will comprise tools

- for rigorous simulation of large hybrid systems consisting of complex switched continuous dynamics and distributed, hierarchically organized supervisory controls defined by intuitive, graphical or textual formalisms
- for model simplification/abstraction which derive consistent over-approximations of complex hybrid dynamic systems for analysis and synthesis purposes
- for the identification of hybrid models from simulated or real data
- for system analysis (e. g. reachability analysis, logic verification), controller synthesis, and on-line optimization of classes of simple hybrid systems
- for real-time simulation for validation by hardware-in-the-loop simulation
- for code generation to test controllers in the implementation environment.

The strategy in HYCON is to provide a set of interchange formats such that the horizontal integration is made as easy as possible. For each tool to be integrated, a translator will be implemented converting into and from the interchange format of the corresponding level of abstraction. This simplifies the model exchange among tools based on similar formalisms and allows supporting specific features that can not be considered in a uniform approach (e.g., based on a single general interchange format). In HYCON three interchange formats are being / have been developed: a format for nonlinear deterministic hybrid models (based on the Matlab S-function interface), one for nonlinear and nondeterministic hybrid models (open issue), and one for switched linear dynamic systems (an XML-representation of piecewise affine dynamical systems). The vertical integration will be realized for these three interchange formats such that the tool developers do not have to worry about problems related to other levels of abstraction.

FORMAL VERIFICATION OF CHI MODELS USING PHAVer

D.A. van Beek[1], K.L. Man[2], M.A. Reniers[2], J.E. Rooda[1], and R.R.H. Schiffelers[1]

[1] Department of Mechanical Engineering, Eindhoven University of Technology,
P.O.Box 513 5600 MB Eindhoven, The Netherlands
[2] Department of Computer Science, Eindhoven University of Technology,
P.O.Box 513 5600 MB Eindhoven, The Netherlands
{d.a.v.beek, k.l.man, m.a.reniers, j.e.rooda, r.r.h.schiffelers}@tue.nl

Hybrid systems related research is based on two, originally different, world views: on the one hand the dynamics and control (DC) world view, and on the other hand the computer science (CS) world view. Clearly, hybrid systems represent a domain where the DC and CS world views meet, and we believe that a formalism that integrates the DC and CS world views is a valuable contribution towards integration of the DC and CS methods, techniques, and tools. The hybrid χ formalism [1, 2] is such a formalism. On the one hand, it can deal with continuous-time systems, PWA/MLD/LC systems, and hybrid systems based on sets of ordinary differential equations using discontinuous functions in combination with algebraic constraints (the DC approach). On the other hand, it can deal with discrete-event systems, without continuous variables or differential equations, and with hybrid systems in which discontinuities take place (mainly) by means of actions (the CS approach). The intended use of hybrid χ is for modeling, simulation, verification, and real-time control. Its application domain ranges from physical phenomena, such as dry friction, to large and complex manufacturing systems. The history of the χ formalism dates back quite some time. It was originally designed as a modeling and simulation language for specification of discrete-event, continuous-time or combined discrete-event/continuous-time models. The simulator was successfully applied to a large number of industrial cases, such as an integrated circuit manufacturing plant, a brewery, and process industry plants [3]. Recently, the χ language has been redefined as a hybrid process algebra with a formal semantics, which enables verification of χ models.

One of the most successful formalisms for hybrid system verification is the theory of hybrid automata. In [2], formal translations between χ and hybrid automata (in both directions) have been defined. The translation from hybrid automata to χ aims to show that the χ formalism is at least as expressive as the theory of hybrid automata. The translation from (a subset of) χ to hybrid automata enables verification of χ specifications using existing hybrid automata based verification tools. In [2] it is proved that any transition of a χ model can be mimicked by a transition in the corresponding hybrid automaton model and vice versa, which indicates that the translation as defined is correct.

To the best of our knowledge, none of the hybrid automata definitions from literature is expressive enough to be used as the target for the translation of hybrid χ. Therefore, the translation uses a target hybrid automata definition, called HA_{u} automata, where the u stands for urgency, that uses features from different hybrid automata definitions.

In this paper, the hybrid automata definition HA_{u} is given as well as the subset of the χ language that is translated. We use the verification tool PHAVer (Polyhedral Hybrid Automaton Verifyer) [4] to show that it is indeed possible to verify properties of χ specifications using an existing hybrid automata based verification tool. For this purpose, we show that the linear hybrid I/O automata that are used as the underlying mathematical model for the verification tool PHAVer are a subclass of the HA_{u} automata. The verification of properties of a χ specification using PHAVer is illustrated by means of an example: the water-level monitor.

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INTERCHANGE SEMANTICS FOR HYBRID SYSTEM MODELS

Alessandro Pinto[1], Luca P. Carloni[2], Roberto Passerone[3], Alberto Sangiovanni Vincentelli[1]

Department of Electrical Engineering and Computer Sciences
University of California at Berkeley, Berkeley CA 94720
apinto,alberto@eecs.berkeley.edu
Department of Computer Science
Columbia University in the City of New York, NY 10027-7003
luca@cs.columbia.edu
University of Trento, Italy
roby@dit.unitn.it

We propose an interchange format for hybrid systems to allow tool interoperability and seamless exchange of information among the hybrid system research community. The need of an interchange format is clear as the tools that have been developed so far use different modelling assumptions and semantics. In our approach, we focus on the semantics of the interchange format as we believe that only using a well-defined semantics will allow developing translation mechanisms from one tool to another that have guaranteed correctness properties. A unique, precise model of computation would make it impossible to support a variety of models that can be radically different. Hence, we use an ``abstract semantics" in the sense that it can be refined to yield any model of computation, or ``concrete semantics", which, in turn, is associated to the existing languages that are used to specify hybrid systems. We show how leveraging its abstract semantics, the interchange format can be used to capture the essential information across different modelling approaches and how such information can be effectively used in the translation process.

Siconos: a software platform for modeling, simulation, analysis and control of non smooth dynamical systems.

V. Acary, F. Pérignon

INRIA Rhône-Alpes - Bipop project

Zirst - 655 avenue de l'Europe

Montbonnot - 38334 Saint Ismier Cedex - France

Phone: +33 (0)4 76 61 52 00 - Fax : +33 (0)4 76 61 52 52

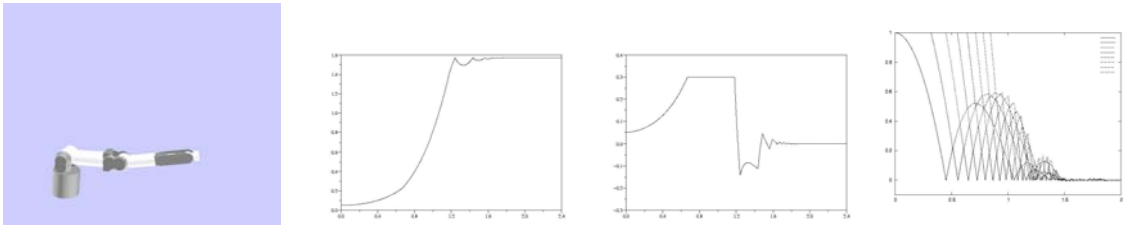
email: vincent.acary@inrialpes.fr, franck.perignon@inrialpes.fr

The first objective of this paper is to give a short overview of what we call Non Smooth Dynamical Systems (NSDS), their link with the hybrid systems framework and what are the benefits of the nonsmooth approach in terms of simulation aspects. Secondly, it aims at presenting the Siconos software, a numerical tool dedicated to modeling and simulation of those NSDS.

Nonsmoothness concerns time-evolution and constitutive equations, in a few words it means that discontinuities can occur in state or time-derivatives. A detailed and complete review on NSDS can be found in [1] and [2]. Typical examples of NSDS are Lagrangian mechanical systems with unilateral contact and friction or linear complementary ones, like electrical circuits including ideal diodes or MOS transistors.

Siconos is a free (GPL GNU license) software[1], dedicated to modeling and simulation of NSDS, in C++ object-oriented language, that allows user to handle various types of dynamical systems, non smooth laws or relations, together with powerful simulation strategies such as time-stepping. Python user interface and XML data management are also available. It thus provides a general and common tool, able to treat problems from different fields (Mechanics, Robotics, Electrical Networks ...). Three typical examples are briefly presented in the full paper. A sample of simulation results is given on Figure 1.

To conclude, a nonsmooth framework permits to precise definitions of solutions together with uniqueness and existence results and the use of specific algorithms (time-stepping, LCP solvers with polynomial complexity) leads to an efficient simulation environment, allowing to treat large dimension problems or systems with impact accumulation.



(a) (b) (c) (d)

Figure 1: (a) robotic arm fall-down - (b) and (c) angular positions of robotic arm parts depending on time - (d) 1000 beads column: vertical displacements of the 8 lowest beads.

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[1] available at `http://siconos.gforge.inria.fr/`

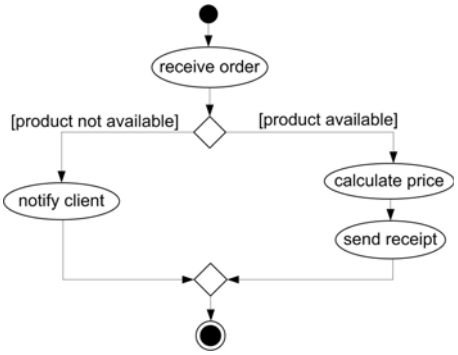
MODELING VISUAL LANGUAGES BASED ON GRAPH TRANSFORMATION CONCEPTS AND TOOLS

Claudia Ermel, Hartmut Ehrig, Karsten Ehrig
Institut für Softwaretechnik und Theoretische Informatik
Technische Universität Berlin, Germany
email:{lieske,ehrig,karstene}@cs.tu-berlin.de

Visual languages (VLs) and visual environments are used in an increasing frequency for software and system development. Prominent examples are the Unified Modeling Language (UML) for software modeling, Petri nets for the design of concurrent system behavior, and a variety of domain-specific diagrammatic notations for various purposes. Although visual languages are used wide-spread, a standard formalism for VL definition such as the Extended Backus-Naur-form (EBNF) for textual languages, is still missing. Nowadays two main approaches to VL definition can be distinguished: grammar-based approaches or meta-modeling. Using graph grammars, multi-dimensional representations are described by graphs and allows not only a visual notation of the concrete syntax, but also a visualization of the abstract syntax. While the concrete syntax contains the concrete layout of a visual notation, the abstract syntax abstracts from the layout and provides a condense representation to be used for further processing. Similarly to the EBNF, rules define the language grammar, but this time, graph rules are used to manipulate the graph representation of a language element.

For the application of graph transformation techniques to VL modeling, *typed attributed graph transformation systems* have proven to be an adequate formalism. Roughly spoken a typed attributed graph transformation rule $p = (L \rightarrow R)$ consists of a pair of typed attributed graphs L and R (its left-hand and right-hand sides). A *direct graph transformation* written $G \overset{p,o}{\Longrightarrow} H$, means that the graph G is transformed into the graph H by applying rule p at the occurrence o of the left-hand side of p in G.

A VL is modeled basically by an *attributed type graph* which captures the definition of the underlying visual alphabet, i.e. the symbols and relations which are available. Sentences or diagrams of the VL are given by attributed graphs typed over the type graph. All concepts and constructions in this paper are illustrated by modeling the VL of activity diagrams, which are used to describe the control flow on activities. A sample activity diagram is depicted to the right.



The abstract alphabet of the sample VL defines two symbol types, *activity* nodes and *next* relations which connect activities. Activities can be of different kinds, i.e. *simple* activities (inscribed by a name), *start* and *end* nodes as well as *decisions*.

The abstract alphabet is extended by defining the concrete layout of activity diagrams. At the concrete syntax level, the VL alphabet defines that an activity is either visualized by an ellipse or by a polygon, depending on the activity kind.

Usually, the set of visual sentences (instances) over an alphabet should be further restricted to the meaningful ones (the valid visual models of the VL). By defining this restriction via graph rules, the constructive way is followed (as opposed to the declarative MOF approach where OCL constraints are used). The application of syntax graph rules builds up abstract syntax graphs of vaild models. Together with a suitable start graph, the set of syntax rules forms the syntax graph grammar which defines the models belonging to a VL in a well-defined and constructive way.

Two tool environments have been developed at TU Berlin to support visual language modeling: the graph transformation engine AGG realizes attributed graph transformation at the abstract syntax level. The visual editor generator Tiger relies on AGG and on the graphical editor framework GEF of Eclipse, and generates a syntax-directed graphical editor from a VL alphabet and a syntax graph grammar. The generated Java code implements an Eclipse visual editor plug-in based on GEF which makes use of a variety of GEF's predefined editor functionalities. Hence, the generated editor plug-in appears in a timely fashion and the generated editor code may easily be extended by further functionalities.

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Mathematical Modelling of Semiconductor Devices

Transparent Boundary Conditions for Quantum-Waveguide Simulations

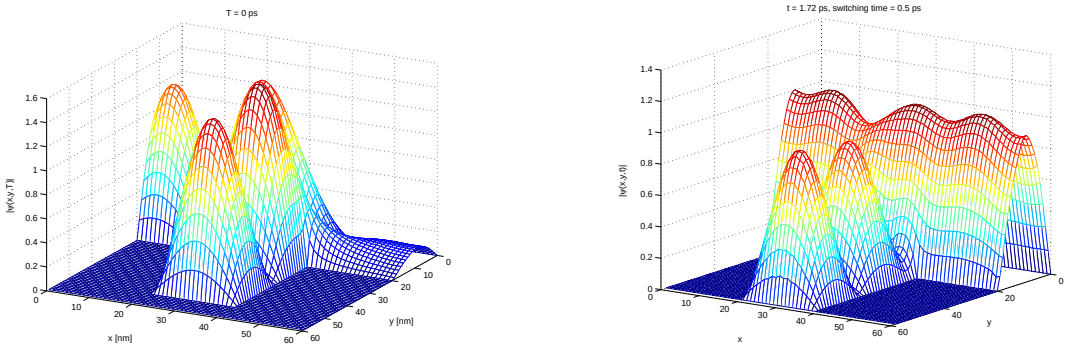
A. Arnold
Vienna University of Technology
Wiedner Hauptstraße 8–10, A-1040 Wien, Austria
Phone: +43 1 58801-10181, Fax: +43 1 58801-10198
e-mail: anton.arnold@tuwien.ac.at

Quantum waveguides are novel electronic switches of nanoscale dimensions. They are made of several different semiconductor materials such that the electron flow is confined to small channels or waveguides. Due to their sandwiched structure the relevant geometry for the electron current is roughly two dimensional. Using external electrostatic potentials the "allowed region" for the electrons, and hence the geometry can be modified. This allows to control the current flow through such an electronic device. It makes it a switch, which resambles a transistor, but on a nano-scale.

Being quantum particles, the electron transport through a quantum waveguide can be modeled in good approximation by a two dimensional, time dependent Schrödinger equation on a time-dependent geometry. This spatial domain consists of (very long) leads and the active switching region, which sometimes has the shape of a stub. In typical applications, electrons are continuously fed into the lead. Depending on the size and shape of the stub, the electron current is either reflected (off-state of the device, see left figure) or it can flow through the device (on-state, see right figure). Since the applied external potential can modify the stub, it hence allows to switch the device.

Important device data for practitioners are the ratio between the on- and the (residual) off-current as well as the switching time between these two stationary states. These data can be obtained from numerical simulations of the described Schrödinger equation model. The leads are very long compared to the typical size of the active region. For the efficiency of numerical simulations it is therefore desireable to restrict this model to a small region close to the stub (see figure). Hence, the leads have to be cut off by using articifical boundary conditions. This is possible without changing the solution of the Schrödinger equation by introducing "transparent boundary conditions" (TBC), which are non-local in time (convolution type) and in space.

The numerical discretizations of these artificial boundary conditions is a main challenge, as it may easily render the initial-boundary value problem unstable. Based on a Crank-Nicolson finite difference discretization of the Schrödinger equation, we shall discuss a dicrete TBC, which makes the overall scheme unconditionally stable. Further, we derive approximations of the involved discrete convolutions by exponential sums, and analyze the stability of the resulting numerical scheme. The derived boundary conditions are illustrated by simulations of a waveguide with a resonating stab.



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MATHEMATICAL MODELLING OF SEMICONDUCTOR-SUPERCONDUCTOR HYBRID STRUCTURES

F. Libisch, S. Rotter, and J. Burgdörfer

Corresponding Author: F. Libisch
Institute for Theoretical Physics, Vienna University of Technology
Wiedner Hauptstraße 8-10/136, A-1040 Vienna, Austria, EU
Phone: +43 1 58801-13612, Fax: +43 1 58801-13699
email: florian@concord.itp.tuwien.ac.at

Modern manufacturing techniques of semiconductor devices allow the study of single electrons confined to two-dimensional cavities, with linear dimension of the order of a micrometer and below. Such devices are typically referred to as "quantum billiards" as the confined electron would classically move like a point-like billiard ball within the two-dimensional potential landscape enclosed by hard-wall boundaries. The stationary states and the corresponding energy eigenvalues of these structures can be obtained by solving the one-particle Schrödinger equation. Because the ensemble of classical periodic orbits determines the quantum mechanical energy eigenspectrum of the billiards, the quantum-to-classical correspondence of the electron dynamics can be probed.

Replacing part of the hard wall boundary by a superconductor (S) gives rise to coherent scattering of an incoming electron into an outgoing hole. This process, generally known as Andreev reflection, connects the electron and hole degrees of freedom at the S boundary. In classical terms, the hole emitted by the S-boundary follows the time-reversed path of the electron. At its next contact with the superconductor the hole is converted back into an electron, thereby forming a periodic electron-hole orbit (see Fig. 1 for illustration). "Andreev billiards" contain a continuum of periodic orbits which leave their mark on the eigenvalue spectrum.

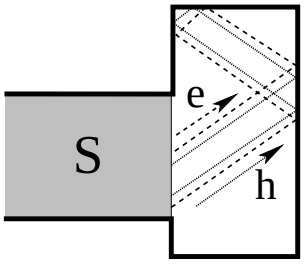

FIG. 1. *Andreev billiard consisting of a rectangular area confined by hard walls and a superconducting boundary (S, shaded).*

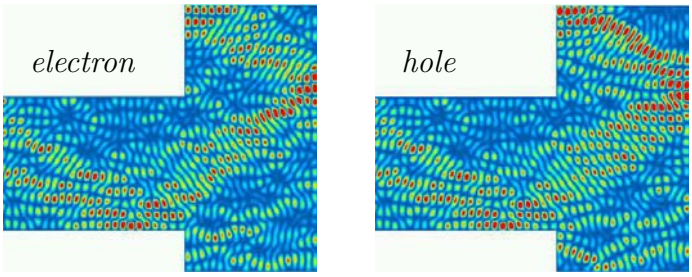

FIG. 2. *The absolute square of electron and hole part of an eigenstate of the Andreev billiard shown in Fig. 1. Note (i) the density enhancements near the semiclassical orbit shown in Fig. 1 and (ii) the similarity between electron and hole wavefunction.*

We report on a detailed investigation on the eigenvalues and eigenstates of the one-particle time-independent Schrödinger equation for Andreev billiards in two dimensions. To solve this elliptical partial differential equation, we use a Green's function approach based on a numerical grid-discretization. We employ Dirichlet boundary conditions at the hard wall boundaries and a wave function matching technique at the S boundary to determine the eigenstates and eigenenergies, [1, 2]. Thereby very accurate solutions for the quantum eigenenergies and the corresponding wavefunctions can be obtained. We find that the eigenenergies can be predicted by a simple semiclassical periodic-orbit quantization scheme based on classical trajectory simulations, [1, 2]. Only small deviations between the semiclassical and the quantum solutions occur which we attribute to diffractive scattering mechanisms. The computed wavefunctions show clear signatures of the Andreev reflection process: (i) the electron and the hole part of the solution are very similar to each other (see Fig. 2) - in analogy to the classical picture of retracing electron-hole orbits. (ii) the wavefunctions show strong density enhancements along the classical electron-hole paths (compare Figs. 1 and 2). (iii) quantizing the classical periodic orbit along which the wavefunction localizes gives the correct eigenenergy of the quantum state.

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KINETIC EFFECTS ON THE TRANSPORT PROPERTIES OF SEMICONDUCTOR DEVICES STUDIED BY DETERMINISTIC SOLUTIONS OF THE BOLTZMANN-POISSON SYSTEM

Ch. Auer and F. Schürrer

Institute of Theoretical and Computational Physics
Graz University of Technology
Petersgasse 16, 8010 Graz, Austria
Phone: +43 316 873–8187, Fax: +43 316 873–8677
email: auer@itp.tu-graz.ac.at, schuerrer@itp.tu-graz.ac.at

In present and forthcoming semiconductor devices, the scale length of individual components is comparable with the distance between successive scattering events of the carriers. An accurate description of the charge transport in such regimes requires treatment within the framework of kinetic theory. Sophisticated kinetic transport models are based on semiconductor Boltzmann equations (BE) coupled with the Poisson equation determining the phase-space distribution of electrons and the electric field in a self-consistent way [3]. The high-field electron transport in polar semiconductors, such as gallium arsenide or indium phosphide (InP), is essentially influenced by the non-equilibrium behavior of polar optical (pop) phonons [1, 4, 6]. Hence, we consider an InP transport model consisting of a coupled set of Boltzmann equations for electrons and pop phonons to take into account the hot-phonon effects dynamically.

So far, mainly stochastic solution methods [5] have been applied to solve the Boltzmann-Poisson system and the coupled kinetic equations of electrons and pop phonons. Recently, efficient deterministic solution methods [2, 4] have been developed as an alternative to the Monte Carlo techniques. These methods are based on full discretizations of the phase space. Conservative finite-difference schemes with shock-capturing reconstructions of the numerical fluxes are applied to approximate the distribution functions accurately even at the junctions of sharp doping profiles [2]. The deterministic approach offers the possibility to directly obtain the distribution functions without statistical noise at computational effort comparable with that of Monte Carlo methods. Hence, the developed numerical techniques allow us to perform detailed studies of the transport properties of sub-micron semiconductor devices in far-from-equilibrium situations.

In this paper, we present transport simulations of spatially one-dimensional device structures. Kinetic effects on the electron transport in a silicon *npn*-structure are studied by comparing the solution of the Boltzmann equation with corresponding maximum entropy distributions, which are used to define closure relations of hydrodynamical transport models. An indium phosphide $n^+ - n - n^+$ diode is considered to investigate the impact of non-equilibrium polar optical phonons on the electron transport. For both devices, the performed analysis of the carrier transport gives evidence that accurate simulations of sub-micron devices should be based on kinetic transport models.

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EFFECT OF BAND STRUCTURE DISCRETIZATION ON THE PERFORMANCE OF FULL-BAND MONTE CARLO SIMULATION

G. Karlowatz, W. Wessner, and H. Kosina, Institute for Microelectronics, TU Vienna, Austria

Corresponding author: G. Karlowatz
TU Vienna, Gusshausstr. 27-29/E360, A-1040 Vienna, Austria
Phone: +43 1 58801-36030, Fax: +43 1 58801-36099
email: gerhard.karlowatz@iue.tuwien.ac.at

Full-band Monte Carlo (FBMC) simulation offers an accurate technique for numerical semiconductor device modeling [1]. A numerical representation of the band structure in the unit cell of the reciprocal lattice, the so called *Brillouin zone* [2], is used. In this work we outline an efficient FBMC simulator and investigate both the accuracy and computional costs of simulation results for two different meshing approaches for the Brillouin zone of silicon.

The first mesh type is based on an octree-based approach. Each cube is split into six tetrahedrons. To mesh a $\{111\}$ surface either one or five tetrahedrons have to be cut away from the six tetrahedrons forming one cube. The result is a structured tetrahedral mesh, whose surface follows exactly the shape of the Brillouin zone. The second mesh type is an unstructured tetrahedral mesh with flexible element grading. It yields a lower total number of tetrahedrons and guarantees a good spatial resolution in regions of interest [3]. The finest resolution is needed around the band minima, because this is the area of the highest electron population, and also the relative error of the linear energy approximation within the tetrahedrons becomes most critical.

Two meshes, a fine one and a coarse one were generated for each the structured and the unstructured mesh type. Figure 1 shows the normalized mean energy of electrons obtained from FBMC simulation at thermal equilibrium. The unstructured meshes are in excellent agreement and converge for low temperatures to the theoretical equilibrium value of $3k_{\mathrm{B}}T/2$. While the fine structured mesh is sufficiently accurate at high temperatures, both structured meshes fail at low temperatures. Figure 2 shows a comparison of simulation results for the velocity as a function of the field for both structured and unstructured tetrahedral meshes. As the curves for 300K and for 77K are grouped very close together above 10kV/cm, it can be concluded that the performance in the high field regime is about the same for all meshes. This result demonstrates that the unstructured meshes perform very well in the high energy regimes, despite they contain less mesh elements than the structured meshes in that areas.

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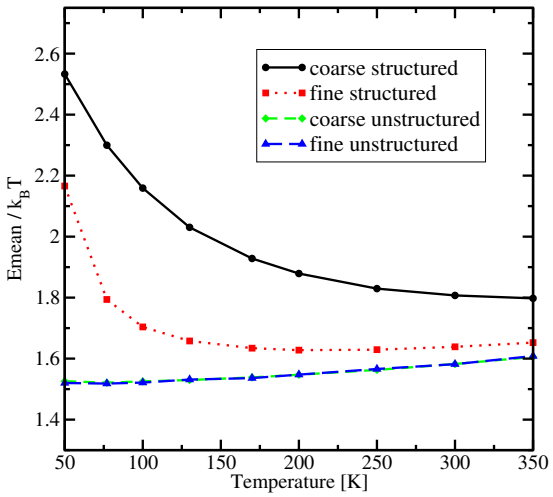

Figure 1: Normalized mean energy of electrons at thermal equilibrium versus temperature.

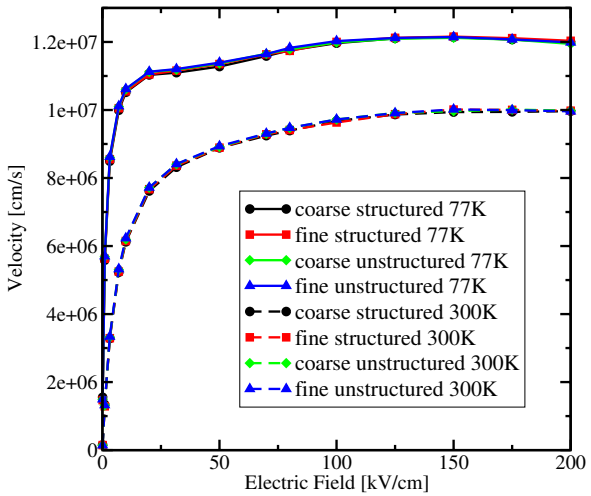

Figure 2: Electron velocity versus field along [100] direction at 77K and 300K.

Simulation of Microelectronic Structures using A Posteriori Error Estimation and Mesh Optimization

Michael Spevak°, René Heinzl△, Philipp Schwaha△, and Tibor Grasser△

Corresponding Author: M. Spevak
°Institute for Microelectronics, Technical University Vienna, Gußhausstraße 27-29/E360, A-1040 Vienna, Austria
△Christian Doppler Laboratory for TCAD in Microelectronics at the Institute for Microelectronics
E-mail: {spevak|heinzl|schwaha|grasser}@iue.tuwien.ac.at

Introduction

Problems occurring in microelectronic device design and TCAD (Technology Computer Aided Design) are often modeled by means of partial differential equations (PDEs). An essential step in all of these methods is to find a proper tessellation of a continuous domain with discrete elements, either based on ortho-product grids or unstructured meshes.

Int. J. Numer. Meth. Engrg. 24 (1987) 337–357. MR 87m:73055 The major advantages of the unstructured mesh approach is that tetrahedral or triangular meshes are locally adaptable and surfaces can be modeled with arbitrary precision. While in two dimensions mesh generation and adaptation techniques are mostly based on hand crafted meshes, it is almost impossible to design and adapt meshes in three dimensions. On that account it is very important to automatically generate and optimize meshes in three-dimensions.

Error Estimation Techniques and Mesh Optimization

As a first step we estimate the error caused by the discretization we have chosen. This may either be a finite volume or finite element discretization. First we will introduce residual error estimators. Due to the discretization the numerical solution does not fulfill the differential equation exactly and therefore the residuum is used as a measure of the discretization error [1]. The ZZ error estimator [2] measures how much the numerical solution u_h differs from a smoothed numerical solution $\overline{u_h}$. For some types of differential equations, such as the Laplace equation, the ZZ estimator has been shown to have upper and lower error bounds [2].

After calculating a local measure for the error we have to adapt the mesh in order to improve the quality of the solution if this measure exceeds an upper limit. On the other hand, we have to coarsen the mesh if the error is smaller than a lower error limit in order not to use unnecessarily fine meshes in regions of low error. The process of inserting more tetrahedra into the mesh is called mesh refinement, removal of elements from the mesh is called coarsement. In the following the complete processes is referred to as mesh adaptation.

There are different techniques of mesh control. The easiest method is to introduce an upper and a lower bound for refinement and coarsement as mentioned before. Second the upper error bound can be set to a level so that a certain number of cells (e.g. the worst 20 per cent) is refined.

Examples and Conclusion

To illustrate the applicability we analyze an interconnect structure by solving the Laplace equation in the SiO_2 layer around the contacts. The main aim of this simulation is to determine the capacitance between the two electrodes both very precisely and efficiently.

Using the advantages of mesh adaptation in combination with a posteriori error estimation leads to an enormous speed up of the calculations while the accuracy of the simulation result is comparable to the uniformly refined and highly resolved solution. For this reason mesh adaptation allows us to improve the mesh quality locally without increasing the number of mesh points dramatically.

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Inverse Dopant Profiling for Highly Doped Semiconductor Devices

Marie-Therese Wolfram
Johann Radon Institute for Computational and Applied Mathematics (ÖAW)
Altenbergerstr. 69, A 4040 Linz, Austria
wolfram.marietherese@oeaw.ac.at

Martin Burger
Industrial Mathematics Institute, Johannes Kepler University
Altenbergerstr. 69, A 4040 Linz, Austria
martin.burger@jku.at

Corresponding Author: Marie-Therese Wolfram

Inverse dopant profiling of devices is a problem of fundamental importance for modern semiconductor technology. Significant subproblems are optimal design for improved manufacturing (cf. [6, 4]) and identification for quality control (cf. [1, 2, 3, 7]).
In this paper we discuss the identification of major features of a doping profile in the case of high doping. This inverse problem is solved using transient measurements of electrical currents and capacitances. The major advantage in the transient setup is the availability of much more data than in the steady state case. Due to the high doping, an assymptotic expansion of the transient drift-diffusion equations is presented, which yields to a reduced model. Using this model we reconstruct major features of the doping profile, namely the values of the donor and acceptor concentration and the value of the junction. We will briefly discuss the underlying analysis and present numerical examples.

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Future Mobile Communication Systems

LOW COMPLEXITY SIMULATION OF WIRELESS CHANNELS USING DISCRETE PROLATE SPHEROIDAL SEQUENCES

Florian Kaltenberger[1], *Thomas Zemen*[2], *Christoph W. Ueberhuber*[3]

[1]Corresponding Author:
F. Kaltenberger
ARC Seibersdorf research GmbH
Donau-City-Str. 1,
1220 Vienna, Austria
E-mail:
florian.kaltenberger@arcs.ac.at

[2]Forschungszentrum
Telekommunikation Wien
Donau-City-Str. 1,
1220 Vienna, Austria
E-mail: thomas.zemen@ftw.at

[3]Vienna University of Technology
Wiedner Hauptstrasse 8-10/101
1040 Vienna, Austria
Email: c.ueberhuber@tuwien.ac.at

Abstract The modeling and simulation of wireless mobile communication channels is very important for the design and testing of receiver algorithms. Especially for the testing of mobile radio hardware devices, real-time implementations of such channel models are required. This work presents a low-complexity algorithm for the simulation of time-variant flat-fading channels. The new method is based on a subspace representation of the channel transfer function. We develop an algorithm to calculate the projection on this subspace in $\mathcal{O}(1)$ operations. By adjusting the dimension of the subspace it is possible to trade complexity for accuracy.

Problem Description The wireless mobile communication channel can be modeled as a linear time-variant system. This system is uniquely characterized using a time-variant impulse response $h(t,\tau)$ where t denotes time and τ denotes the time delay of the impulse response. Complex symbols are transmitted over the channel at rate $1/T_{\mathrm{S}}$. If the symbol duration T_{S} is much longer than the support of the impulse response T_{D}, the channel is called *frequency-flat*. In contrast to block fading channels, where the impulse response is assumed to be constant over a certain time, *time-variant* channels change from symbol to symbol.

Looking at the far field only, and assuming plane waves which are scattered at objects, the time-variant flat-fading channel is modeled using ray tracing principles [1]. Such a channel model has a high computational complexity, because for every propagation path and every time instance a complex exponential has to be evaluated. On a real-time hardware channel simulator, like the *ARC SmartSim* [2], the number of paths P, that can be simulated, is limited by the available processing power. In this paper, a new method is introduced, that allows both to increase the number of paths P and to reduce the overall computational complexity.

Contributions

- The subspace representation of a time-variant channel from [3] is applied to time-variant channel *simulation*.
- Approximate DPS wave functions are introduced, that allow to calculate the projection on the subspace in $\mathcal{O}(1)$ operations.
- A detailed error and complexity analysis that allows to trade efficiency for accuracy is provided.

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TIME-VARIANT CHANNEL PREDICTION USING TIME-CONCENTRATED AND BANDLIMITED SEQUENCES - ANALYTIC RESULTS

Thomas Zemen[1], *Christoph F. Mecklenbräuker*[1] *and Bernard H. Fleury*[2]

[1]Corresponding Author: T. Zemen
Forschungszentrum Telekommunikation Wien
Donau-City Str. 1/3,
1220 Vienna, Austria
E-mail: {thomas.zemen, mecklenbraeuker}@ftw.at

[2]Aalborg University
Fredrik Bajers Vej 7-A3
9220 Aalborg, Denmark
Email: fleury@kom.aau.dk

Abstract We use time-concentrated and bandlimited sequences for minimum-energy prediction of time-variant flat-fading channels. The time-concentration of these sequences is matched to the length of the observation interval and the band-limitation is determined by the Doppler bandwidth of the time-selective fading process. We prove in this paper that minimum-energy bandlimited prediction is identical to reduced-rank maximum likelihood filtering (which is a close approximation of Wiener filtering). In wireless communication systems the time-selective fading process is highly over-sampled. Thus the essential dimension of the subspace spanned by time-concentrated and bandlimited sequences is small. The prediction error mainly depends on the Doppler bandwidth, while the actual shape of the Doppler spectrum is of minor importance. Analytic performance results prove this fact for a practical wireless communication system.

Problem Description The Doppler bandwidth in wireless communication systems is much smaller than the actual channel bandwidth. We exploit this basic fact for minimum-energy bandlimited prediction of a time-variant flat-fading channel by using a low dimensional subspace spanned by time-concentrated and bandlimited sequences [1]. The time-concentration of these sequences is matched to the length of the observation interval and the band-limitation is chosen according to the Doppler bandwidth of the time-selective fading process. We present analytic performance results and highlight the tight interconnection of minimum-energy bandlimited prediction to linear minimum mean square error (MMSE) channel prediction [2, Section 12.7].

In wireless communication systems the normalized Doppler bandwidth $\nu_{\mathrm{D}} \ll 1/2$. In this case the time-variant channel coefficients can be described using a subspace representation with extremely small dimensionality [3]. In other words, the detailed shape of the Doppler spectrum is of minor importance. Only the Doppler bandwidth ν_{D} and the observation interval length M are the prime parameters that define the subspace dimension $D' = \lceil 2\nu_{\mathrm{D}} M \rceil + 1$. This result is utilized for time-variant channel *estimation* in [4]. In the present paper we extend the concept to time-variant channel *prediction*.

Contributions

- We present analytic performance results for minimum-energy bandlimited prediction of time-variant flat-fading channels.
- We show that minimum-energy bandlimited prediction is equivalent to reduced-rank maximum likelihood (ML) filtering. Reduced-rank ML filtering itself is a close approximation of linear MMSE (Wiener) filtering. This result allows to clarify the strictly limited prediction horizon of linear prediction techniques.

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ADVANCED MATHEMATICAL MODELS FOR THE DESIGN AND OPTIMIZATION OF LOW-INTERFERENCE WIRELESS MULTICARRIER SYSTEMS

G. Matz[a] (corresponding author), K. Gröchenig[b], F. Hlawatsch[a], A. Klotz[b], G. Tauböck[a], and A. Skupch[a]

[a]Institute of Communications and Radio-Frequency Engineering, Vienna University of Technology
Gusshausstrasse 25/389, A-1040 Vienna, Austria
gmatz@nt.tuwien.ac.at

[b]Faculty of Mathematics, University of Vienna
Nordbergstrasse 15, A-1090 Vienna, Austria

We apply frame theory and related mathematical models and results to multicarrier (MC) communication systems with pulse shaping and transmission over doubly dispersive fading channels (e.g., [1–4]). Expressions for the intersymbol and intercarrier interference (ISI/ICI) occurring in such systems reveal that the time and frequency concentration of the transmit and receive pulses is of paramount importance for low ISI/ICI. We prove the existence of such jointly concentrated pulse pairs (cf. also [2]) by adapting recent mathematical results on Weyl-Heisenberg (Gabor) frames [5] to the MC context. Furthermore, we propose pulse optimization procedures that exploit the design freedom existing for redundant MC systems to minimize ISI/ICI. Simulation results demonstrate that our optimized pulse-shaping MC systems can outperform conventional cyclic-prefix OFDM systems for realistic system parameters.

The following topics are covered in detail:

- A signal and transceiver model for MC systems using a Gabor Riesz sequence.
- A nearly diagonal model for dispersive fading channels.
- Mathematical models for the design of transmitter/receiver pulses: The *Ron-Shen duality* [6] allows the use of well established Gabor-frame methods [7] for the construction of Gabor Riesz sequences or even orthonormal Gabor systems. It is thus possible to transfer recent mathematical results [5] on the time-frequency localization of Gabor frame atoms to the transmitter/receiver pulses of MC systems.
- An analysis of the mean ISI/ICI power of pulse-shaping MC systems transmitting over a *wide-sense stationary uncorrelated scattering* (WSSUS) [8, 9] channel (cf. also [3]).
- Two methods for designing optimal transmit and receive pulses with minimum ISI/ICI power.
- An experimental assessment of the superior performance of optimized pulse-shaping MC systems.

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A REALISTIC RADIO CHANNEL MODEL BASED ON STOCHASTIC PROPAGATION GRAPHS

Troels Pedersen and Bernard H. Fleury

Aalborg University, Institute of Electronic Systems, Information and Signals Division,
Frederik Bajersvej 7A, DK-9220, Aalborg East, Denmark.
email: troels@kom.aau.dk

The design and optimisation of modern radio communication systems require realistic models of the radio propagation channel, which incorporate dispersion in delay, Doppler frequency, direction of departure, direction of arrival, and polarisation. Often radio communication systems are assessed by Monte Carlo simulations in which stochastic models are used to generate synthetic realisations of the response of the radio channel.

Traditional stochastic radio channel models reflect the statistical properties of the (time-variant or time-invariant) impulse response of the channel between the input of any antenna element at the transmitter site and any antenna element at the receiver site. The probability distributions of the parameters of the channel impulse response are generally difficult to obtain from environment parameters such as the scatterer size and density. Instead, the model parameters are often inferred from measurements. Motivated by experimental results conventional models implement an exponentially decaying power-delay-profile by including various ad-hoc constraints on the random model parameters. These approaches, however, do not reflect the underlying physical mechanisms that lead to this decaying behaviour.

In this contribution we present a stochastic model of the radio propagation environment based on a random propagation graph. A propagation graph is defined by a set of vertices (the transmitter, the receiver and the scatterers) and a set of edges (visibility between scatterers). The position of the scatterers and the edges of a propagation graph are drawn randomly according to some probability density functions.

The propagation process is modelled as follows. The transmitter vertex emits an electromagnetic signal illuminating a subset of the vertices. As a signal propagates along an edge of the propagation graph, it is delayed and attenuated depending on the length of the edge. When the signal arrives at a scatterer it is re-radiated by the scatterer. The interaction between the signal and a scatterer is modelled as a scatter-gain weighting all signals arriving at this scatterer. From a realisation of the propagation graph the received signal of a specific communication system can be computed.

Simulations show that under the assumption of an inverse squared distance power decay, the proposed model yields the often observed exponentially decaying power-delay-profile. This effect stems from the structure of the propagation graph and is not obtained by introducing any artificial constraints. The channel realisations obtained from the model also exhibit a transition from specular contributions for small delays to a diffuse part at long delays with a mixture of specular and diffuse contributions at intermediate delays. This feature is also observed experimentally, especially in investigations for ultra wide band systems. The model for the power-delay-profile can be easily extended to include dispersion in direction of departure and direction of arrival.

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MAXIMUM ENTROPY MIMO WIRELESS CHANNEL MODELS WITH LIMITED INFORMATION

M. Guillaud and M. Debbah, Eurecom Institute, France

Institut Eurécom, Mobile Communications Department
2229 Route des Crêtes, 06904 Sophia-Antipolis, France
Phone: +33 4 93 00 81 37, Fax: +33 4 93 00 26 27
email: {guillaud,debbah}@eurecom.fr

Abstract

In this contribution, analytical wireless channel models are derived from the maximum entropy principle [1], when only limited information on the environment is available. The method outlined in [2] is applied to situations where analytical models of the fading characteristics of a multiple-antennas wireless channel are needed, and where the classical Rayleigh fading model is too coarse.

The issues of the knowledge of the average channel energy, of an energy upper-bound, and of spatial correlation, are studied. First, analytical models are derived for the cases where these parameters are known deterministically. Frequently, these parameters are unknown, but still known to represent meaningful system characteristics (this includes typical scenarios where the received energy or the spatial correlation varies with the user position). In these cases, consistent analytical channel models are derived, based on maximum entropy distributions of the energy or space correlation parameters.

For the unknown energy case, we derive a model under energy average and upper-bound constraints intended to model the effects of shadowing. This model is compared in terms of mutual information to the classical i.i.d. Gaussian model in the SISO case. Numerical simulations show that the proposed model exhibits a reduced outage capacity w.r.t. the known energy case.

When the spatial covariance matrix is unknown, but is known to be a preponderant parameter, we derive a model by first maximizing the entropy of the covariance matrix, and then marginalizing. We show that this situation is conveniently handled through the eigenvalues of the covariance matrix, whereas its eigenvectors are uniformly distributed. Using this technique, the modeler can provide consistent models incorporating correlation of the channel antenna gains without the explicit value of these gains.

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Adaptive algorithms for mobile digital signal transmission *

Massimo Fornasier
NuHAG, Fakultät Mathematik
Universität Wien
Nordbergstrasse 15
A-1090 Wien
email: mfornasi@math.unipd.it

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Abstract

This contribution is concerned with wireless digital signal transmission [7]. The transmission of a signal through a wireless channel is modeled as the action of a pseudodifferential operator with symbol in certain symbol classes [6, 2, 3, 4, 5]. In fact, due to possible different spatial paths done by the signal and possible frequency delays due to Doppler effects, the received signal r can be expressed as a superposition of amplitude modulated time-frequency shifts of the original signal s. The amplitudes are governed by the symbol σ of the operator.

$$r(t) = T_\sigma s(t) = \int_{\mathbb{R}} \int_{\mathbb{R}} \sigma(x,\omega) e^{2\pi i \omega t} s(t-x) dx d\omega$$

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Mathematical Models of Co-operative Multiagent Systems

INDUSTRIAL APPLICATIONS OF ROBOTSOCCER

P. Kopacek, TU Vienna, Austria

Corresponding Author: P. Kopacek
Intelligent Handling and Robotics
Vienna University of Technology
Favoritenstraße 9-11, 1040 Wien, Austria
Phone: + 43 1 58801-31801, Fax: + 43 1 58801-31899
email: kopacek@ihrt.tuwien.ac.at

Robot soccer was introduced with the purpose to develop intelligent cooperative multi-robot (agents) systems (MAS). From the scientific point of view a soccer robot is an intelligent, autonomous agent, carrying out tasks together with other agents in a cooperative, coordinated and communicative way. Robot soccer provides a good opportunity to implement and test MAS algorithms. One of the newest approaches in robotics is the application of robots in entertainment, leisure, hobby and education. A new term "edutainment" – composed of two words, education and entertainment, is widely spread. Robot soccer is a good tool to teach people the complicated technical knowledge in the way of playing.

In this presentation industrial applications directly derived from robot soccer will be described.

Our semiautomatised disassembly cell for handies consists of five automated stations plus a manual feeding and removal station. Before the mobile phone is fixed on a pallet the power supply will be removed and the type of the handy will be recognized by a barcode reader manually. Now the control computer knows exactly the type of the handy and the main dimensions. In the drilling and milling station the upper part of the handy will be cut off from the lower part and the screws are removed by a simple drilling mechanism. In the cover removal station – the cover as well as the keyboard of the handy will be removed by pneumatic sucks and in the drilling station – the screws which connect the printed circuit board to the lower part of the housing are removed. Because the screws of the handies have a diameter of 1.25mm a very accurate image processing system is necessary. With our system from robot soccer we reach very good results.

To get energy from the sun an approach is to set up nets with solar cells in the space and transmit the energy wireless to the earth by microwaves. For first tests a net (approximately 40 x 40 m) equipped with solar cells should be installed in outer space (~ 200 km above the earth). The main problem is the positioning of the solar cells on the net structure. For this task autonomous mobile robots could be used able to move (crawl) on this large quadratic mesh. The distance of the mesh wires is between 3 and 5cm; their thickness between 1 and 3mm.

The features of an autonomous mini robot for this purpose are: the maximum dimension 10x10x5cm, light weight (less than 1 kg), "low cost", on board power supply for approximately 10min, equipped with a camera sending pictures to the earth, wireless communication with the mother satellite by Bluetooth or similar, mechanical and electronic robustness against low/high temperature, radiation, microgravity, vibration and shock during the flight in the rocket.

As a direct spin off from robot soccer three prototypes - Roby-Sandwich, Roby-Insect and Roby-Junior, based on "Roby-Speed" - were developed. In January 2005 these three robots were tested in the micro-gravity environment by means of parabolic flights in Japan.

TRANSFORMED NET – COLLISION AVOIDANCE ALGORITHM FOR ROBOTIC SOCCER

Martin Saska, Miroslav Kulich, Gregor Klančar, Jan Faigl

Corresponding Author: Martin Saska
Phone: (+420)224355765 Fax: (+420)224 357 224
email: saska@labe.felk.cvut.cz

Fast and robust obstacle avoidance plays an important role for design of a successful robot soccer team, although not all teams use it nowadays. Many different algorithms for obstacle avoidance were mentioned in the standard robotic literature. Unfortunately, these approaches cannot be directly used for robot soccer due to several reasons. The standard algorithms assume that a working environment is static or changing slowly. Moreover, computation time and time needed for realization of the planned path is usually not crucial. On the other hand, a robot soccer environment is highly dynamic. Speed of robot soccer players (which act as obstacles) can be several meters per second, what requires low reaction time. While movements of teammates are known (all members of one team share the same information), opponent players' behavior is hard to predict. One criterion for obstacle avoidance is therefore to plan a path far enough from opponent robots to guarantee that their trajectories will not collide with the planned one. This is in contradiction to a primary goal of robot soccer – to reach the ball as fast as possible (or faster than opponents at least) in order to score a goal or defend the opponent to score. An obstacle avoidance algorithm suited for robot soccer should find acceptable compromise between these two antagonistic requirements.

The novel obstacle avoidance algorithm – transformed net satisfying the above-mentioned criteria is introduced in the paper. The approach constructs a grid of points covering an area along a straight line connecting robot's actual position with a requested goal position. The points in the grid are connected so that they form a plannar graph. A number of points in the net depends on the distance between the start and goal position. In order to increase a speed of the algorithm, the net is not computed on the fly. Instead of this, several basic nets with a different number of points are pre-computed. The appropriate net is then chosen in a planning phase and transformed (rotated, shifted, and resized) to a correct position. Edges of the transformed net are evaluated respecting Euclidean distance between points they connect as well as their distance to obstacles (other robots). The final step of the algorithm is to find the cheapest path in the net connecting the start and goal positions. This is done using standard Dijkstra algorithm [1]. The output of the proposed obstacle avoidance algorithm is a sequence of strategic points to be passed through in order to avoid obstacles. A trajectory generator produces feasible and smooth reference path from this set of points. The robot is then controlled using a classic state space controller to follow a preplanned collision free path.

The trajectory generator defines a reference path among those strategic points represented as a smooth path - spline composed of cubic polynomials. The two-dimensional curve is obtained by combining two splines, $x(u)$ and $y(u)$, where u is the parameter along the curve. Each spline consists of more segments - cubic polynomials where knots are points of tangency of two neighboring segments with continuous (same) derivatives. When the knots are set, spline parameters are obtained by solving a linear equation system. A reference velocity profile has to be determined along the obtained path. If the task is to arrive to the final position as soon as possible then maximal allowable velocity profiles that mobile robots could still afford due to acceleration limits is determined as explained in [2]. In the presented paper this velocity profile is fixed, which allows fair comparison of proposed obstacle avoidance method (transformed net) with other standard approaches. Control of the robot on the reference path is done using a well-known approach [3] with combination of feedforward and closed-loop actions. The former uses robot inverse kinematics to calculate the feedforward inputs from the reference curve, while the latter one cancels the effects of noise, disturbances and initial state errors using state space controller.

The above mentioned obstacle avoidance algorithm has been extensively tested on a simulator as well as with a real robot soccer system and compared with two standard approaches – potential field and visibility graph [4].

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DECISION SUPPORT BY SIMULATION IN A ROBOTIC SOCCER DOMAIN

T.Krajník, J.Faigl, L.Přeučil, CTU Prague, Czech republic

Corresponding Author: T.Krajnik
Czech Technical Univeristy in Prague
Technická 2, 16627 Prague 6, Czech Republic
Phone: +420 224 35 5765, Fax: +420 224 35 7224
email: tkrajnik@labe.felk.cvut.cz

The aim of this paper is to present a decision support system for robotic soccer. In a software system managing robots during a soccer match, this component acts as an information provider for other system components. The core of this decision support system is a physics simulator, which can predict game situation. This can be used to predict positions of objects at the moment, when a particular decision takes effect, thus compensating negative influence of transport delays originating in the system. The predicting capability can be also utilized to support tracking algorithms of a vision module. Using an independent information provider has also major impact on overall system architecture, because it shadows limitations imposed by hardware and enables particular system modules to work asynchronously. Important contribution of this component is a strategic decision support by in-game feasibility testing of proposed actions, which is done by evaluating the outcome of a desired action by physical simulation. Moreover, testing of reasoning and control algorithms on a virtual or semi-virtual system is also made possible by this support module.

Classical robotic system [1,2,3] uses a closed loop approach, where commands sent to robots are generated from actual and desired playfield state by sequence of algorithms, which are executed every time an image of the playfield is captured and processed. Since desired state is characterized only by ball position, the first computational step, (mostly called reasoning algorithm) usually covers generating required positions of robots. In the following step (the control algorithm) robot commands are calculated in order to move the robots towards these positions. While the control part is subject to control theory with a well-elaborated mathematical background, rules utilized by strategic planning mostly originate from human soccer tactic and experience gained by previous robosoccer matches.

In our approach, all above-mentioned components (the vision, reasoning and control) work independently of each other. All information about the state on the playfield, i.e. positions and speeds of all objects and intentions of robots, is contained within the support module. This module is capable of predicting future situation as well as updating it from non-actual information. When a particular module provides or requests information about game state, it supplies a timestamp to specify the time validity of this data. To support its tracking and recognition algoritmhs, vision module announces the time of image capture and obtains an estimation of objects positions at that time. The control module estimates the time, when it will transmit orders to the robots and uses predicted positions and speeds to calculate those commands. The reasoning component can set up a set of hypothetical situations called "reasoning frames", which are then simulated to ascertain their feasibility. The best achieved situation is then chosen for execution.

The proposed decision support system was implemented and tested within the MiroSot robosoccer domain of the organization FIRA. Presented solution improves recognition capability of relatively slow vision system (15 fps ~ 66 ms loop) and enables the control system to run in a 20 ms loop with a transport delay about 6 ms. Several cases of reasoning frames usage to determine feasibility of desired actions were also performed.

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An Industrial Image Processing System for Fast Moving Objects

P. Kopacek, M.-W. Han, B. Putz, E. Schierer, M. Würzl
Institute for Mechanics and Mechatronics
Division for Intelligent Handling and Robotics (IHRT)
Vienna University of Technology
Favoritenstr. 9–11, A–1040 Vienna
Tel: +43-1- 58801 31801, FAX: +43-1- 58801 31899
e-mail: kopacek@ihrt.tuwien.ac.at

Abstract. Robot soccer is a good opportunity to implement and test the cooperative group behavior of mobile robots. Basically such a soccer playing team of autonomous robots form a multi agent system (MAS). To individually control each of the robots of a team you can either define a central observing entity which keeps track of the situation on the playground or implement proper control algorithms on each robot in a way that it performs a self-determined intelligent behaviour .

This paper depicts the vision system used in the FIRA MiroSot and NaroSot league. which must be considered both in developing adequate vision algorithms and strategies for game play based on current states of team members and (optionally) position of opponents and the ball as well as the communication module used for transmitting commands to each robot.

Since the robots in FIRA MiroSot and NaroSot evolves more and more faster and quicker the vision system as an integral part of the control loop also must become as fast as possible. The new software of *RobySpeed* and *RobyNaro* consists of a vision system, a communication module and a game strategy module. For the new system our robots were completely redesigned to fulfill the increasing mechanical requirements regarding speed with the arising possibility of heavy collisions. The focus of the software development was on the implementation of the vision system with based on a a digital camera. The most substantial part of the system is to detect the positions of all relevant objects on the playground by analyzing color information. These are first of all own robots (up to eleven in large league) and the ball. If the processing power of the host computer is sufficient also all the hostile robots can be involved in the detection process which (typically) dramatically improves the overall game play. Due to noise effects in the camera‘s sensor chip the probability of erroneous color detection is very high. To eliminate this so-called „salt and pepper“ noise extensive filter operations are performed on the raw image data which make demands on the vision processing time slot.
Further enhancements of the new systems are full pictures instead of half pictures as well as a lower system load on the host computer. Due to its open system architecture it is open for future extensions. Two color models, RGB and HSL were implemented to easily adapt to certain environmental conditions. HSL is particularly suitable for the non-uniform lighting conditions normally found on playgrounds but computationally intensive while RGB, on the other hand, is very easy to implement and fast in computation but not appropriate for most conditions.

The second part of this paper discusses the communication between the soccer robots and the host computer. Depending on the current situation on the playground it selects an appropriate strategy, calculates suitable movement commands and sequentially broadcasts them to each team member. The protocol itself is designed to be unidirectional, implements error correction properties and is optimized to handle up to 11 robots.

LOCALISATION OF MOBILE ROBOTS BY TRACKING IDENTICAL COLOUR MARKERS

G. Klančar[1], M. Brezak[2], I. Petrović[3] and D. Matko[4]

[1,4]Faculty of Electrical Engineering, University of Ljubljana, Slovenia
[2,3]Faculty of Electrical Engineering and Computing, University of Zagreb, Croatia

Corresponding Author: G. Klančar
Faculty of Electrical Engineering, University of Ljubljana
Tržaška 25, SI-1000 Ljubljana, Slovenia
Phone: + 386 2 4768764, Fax: + 386 1 4264631
email: gregor.klancar@fe.uni-lj.si

A reliable tracking algorithm of multiple mobile robots is addressed in this paper. A central vision system (see Fig. 1) is used to find robots in the environment where robots are marked with identical colour patches mounted on each of them. To distinguish robots a robust tracking algorithm considering robot kinematics is implemented.

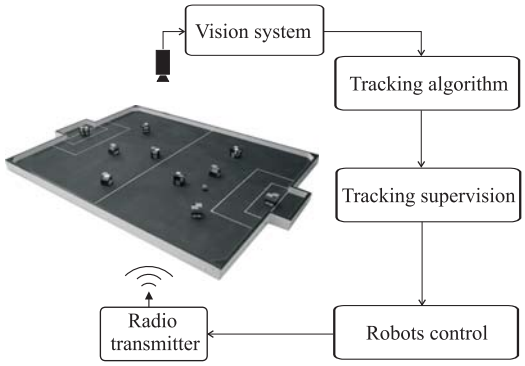

Fig. 1: System overview

Collisions and other unpredictable situations, such as lighting conditions that arise during robots operation or wrong initialisation of robots identifications, can lead to mistakes in the tracking process. Because these mistakes happen rarely, this problem has not been addressed in previous works. However, mistakes such as swaps of robots identifications can happen and are unrecoverable, resulting in wrong control. The control algorithm will not drive these robots correctly because positions estimated by vision system do not belong to these robots but had previously been swapped. This is why this kind of situation has to be detected rapidly in order to apply a different strategy that ensures the continuity of the tracking. In the paper the swaps of robots identifications and initialisation problems are tackled using the supervision algorithm which is based on the correlation of command, and estimated robots velocities.

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Poster Session

ARTERIAL PRESSURE MODELING BY AN INTEGRABLE APPROXIMATION OF NAVIER-STOKES EQUATIONS

T.M. Laleg, E. Crépeau and M. Sorine

Corresponding Author : T.M.Laleg
INRIA Rocquencourt
78153 Le Chesnay cedex, France
Phone :+33 1 39635758, Fax :+33 1 39635786
email :Taous-Meriem.Laleg@inria.fr

Many studies have been devoted to modeling the systemic circulation in order to understand and assess the behavior of the circulatory system both in normal and pathological conditions. One can distinguishes two approaches for modeling the arterial blood pressure (ABP) in large arteries : Lumped models and distributed models. The former which include the famous two, three and four elements windkessel models are $0D$ models. They are based on an analogy with simple RLC electrical circuits [3]. They successfully explain the diastolic phase but, with their low order, they can not explain propagation phenomena like the transit delay of the pressure pulse. On an other hand, distributed models take into account spatial and time variables. The $3D$ models are based on computational fluid dynamic principles and can explain observed phenomena [2]. Too complex for some applications, they can be reduced to $2D$ or $1D$ models. During the propagation of the Pressure Pulse (PP) along the arterial tree, phenomena like "Peaking" and "Steepening" are observed. These have been explained by the linear superposition of direct and reflected harmonic waves, the reflected waves being created when the forward waves, from the heart to the periphery, encounter discontinuities in the arterial properties like a bifurcation or a stenosis. This model has been well known for decades and many studies have been carried out in order to separate the PP into its forward and backward components, as in the pioneering work of Westerhof [4]. Instead of this usual decomposition of the ABP, we suggest to use a nonlinear superposition of forward solitary waves completed by a windkessel flow. The former takes into account fast phenomena which predominate during the systolic phase and the latter represents slow phenomena during the diastolic phase. The introduction of forward solitons explains the "Peaking" and the "Steepening" phenomena. Solitons possess an analytical expression which leads to a reduced ABP model. So, we start from a quasi-one dimensional Navier-Stokes equation to derive a Korteweg-de Vries (KdV) equation which has as particular solution solitons [1], [5]. From real data it seems that a 2 or 3 interacting solitons are sufficient for a good description of the systolic phase. The following figures illustrate satisfactory results obtained from real ABP data measured at the finger level with a FINAPRES. Unlike, the linear approach, which necessitates simultaneous blood pressure and flow measurements, the proposed model requires only pressure measurements. It depends on few number of parameters and it seems that these results on ABP waveform analysis, in particular in the systolic phase, can lead to some interesting clinical applications.

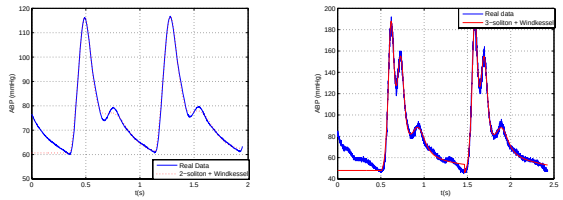

FIG. 1 – Pressure at the finger : real and estimated data

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MODELLING THE MIGRATION OF TRANSURANIUM ELEMENTS IN CONTAMINATED SOILS

Katharina Breitenecker, Helmuth Böck, Mario Villa, Atomic Institute of the Austrian Universities, Austria
Alexander Brandl, Nuclear Engineering Seibersdorf GmbH, Austria

Corresponding Author: Katharina Breitenecker
Atomic Institute of the Austrian Universities
Stadionallee 2, 1020 Wien, Austria
email: Katharina.Breitenecker@ati.ac.at

The radioactive contamination of soils by transuranium elements and their migration paths through the ground is of special interest for this PhD-project. According to the International Atomic Energy Agency (IAEA), who has developed guidance material for site characterization of sites containing radioactive material, known radioactive contaminations are to be investigated for their spatial extent and depth of penetration into the soil. Before remediation activities are designed, the exact boundaries of the contamination and the activity concentration have to be determined.

For this purpose measurement of transuranium elements by in-situ methodologies is challenging at best. Thus, the most commonly used methods include sampling and laboratory analyses, either by alpha spectrometry or liquid scintillation counting. But the costs for these laboratory analyses are high and systematic sampling can be difficult and time consuming.

Therefore a mathematical model that describes the migration of transuranium elements and includes the local topography of the contaminated site and meteorological data shall be established. The idea is to find a mathematical function that is able to determine the contamination of a probably contaminated site, when only a few samples are taken, also with respect to the local parameters mentioned above. For this reason the pathways of these radionuclides from the release point are described by two methods, on the one hand by cellular automata and on the other hand by Monte Carlo simulation.

Cellular Automata: In the middle of a contaminated site an activity of transuranium elements was released into the ground. Under the assumption that migration of these elements could have only taken place by diffusion, the diffusion equation was replaced by a simple discretization for the existing problem and thereafter implemented in MATLAB.

The contaminated site is divided in a regular grid of *cells*, each in one of a finite number of *states*, i.e. from intense contamination to none contamination. Time is discrete, and the state of a cell at time *t* is a function of the states of the *neighborhood-cells* at time *t-1*. That means, if the surrounding neighbour-cells of a certain cell X contain some contamination, than cell X will have some contamination after the next time step, too.

Monte Carlo Simulation: The other version to understand the migration of transuranium elements was done by Monte Carlo Simulation. Therefore, a random walk was implemented in MATLAB.

Future Prospects
The moment the weather becomes drier and clearer, samples have to be taken from the contaminated site to achieve data for the verification of these two models. At the moment it cannot be said which of those suits the migration of transuranium elements in soils best. Therefore analytical data from the contaminated site is necessary for validation.
In the next steps, the dispersion via diffusion equation plus transport equation shall be taken in regard, as well as the radioactive decay of the related transuranium elements. Both, high-pressure-weather and low-pressure-weather influence diffusion differently, and shall therefore be examinated carefully. Furthermore, the slightly different chemical behaviour of different transuranium elements (i.e. uranium, neptunium, plutonium and americium) and the diverse solubilities in different acids will be considered.

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SYNTHESIS OF EXTERNAL LOAD MODEL UNDER UNCERTAINTIES

Yu. Menshikov, DNU, Dnepropetrovsk, Ukraine

Corresponding Author: Yu. Menshikov
Dnepropetrovsk University
Nauchnaja st. 13, 49050, Dnepropetrovsk , Ukraine
Phone: +38 0562 46 00 91, Fax: + 38 0562 4655 23
email: du-mmf@ff.dsu.dp.ua

Abstract. A problem of a correct choice of mathematical model of external load arise often at mathematical modeling of motion of open dynamic systems. One of possible methods of the solution of this problem is identification method [1,2]. In many cases a problem of a finding of mathematical model of external load z can be reduced to a obtaining of the solution of the linear equation

$$A_p z = u_\delta = B_p x_\delta, \tag{1}$$

where z is the function to be found ($z \in Z$), $u_\delta \in U$, x_δ – the given function, ($x_\delta \in X$); A_p, B_p – linear operators, $A_p : Z \to U, B_p : X \to U$; X, Z, U – functional Banach spaces.

The function x_δ is obtained from experiment with a known error δ: $\| x_\delta - x_T \|_X \le \delta$, where x_T is an exact response of object on real external load. The operators are not determined exactly and can be elements of classes $A_p \in K_A, B_p \in K_B$. All operators A_p, B_p have identical structure and differ only with sizes of some parameter $p \in R^n$. The operators A_p are completely continuous, operators B_p are irreversible and linear. By virtue of uncertainties of the mathematical description we shall believe, that the vector p belongs to some closed limited domain $p \in D \subset R^n$. The solution of the equation (1) under the given conditions is an ill-posed problem [3].

Let's consider problem of synthesis of external load model $z^{un} \in Z_1$ which provides the best results of mathematical modeling uniformly for all operators $A_p \in K_A, B_p \in K_B$:

$$\| A_p z^{un} - B_p x_\delta \|_U \le \inf_{z_a} \sup_{p \in D} \| A_p z_a - B_p x_\delta \|_U, \tag{3}$$

where z_a is the solution of extreme problem

$$\Omega[z_a] = \inf_{z \in Z_1 \cap Q_{\delta,a}} \Omega[z],$$

$Q_{\delta,a} = \{ z : z \in Z_1, \| A_a z - B_a x_\delta \|_U \le \| B_a \| \delta, a \in D \}$, $\Omega[z]$ is the stabilizing functional defined on Z_1; Z_1 is everywhere dense set in Z [3].

Let us name function z^{un} as *unitary mathematical model of external load for classes* $\hat{E}_A$, $\hat{E}_B$.
The unitary mathematical model will be additional stable to change of the not taken into account factors [4].
In work was shown that the unitary model exists and is steady to small changes of the initial data.
The offered approach to mathematical models synthesis of external load on dynamical system can find application in cases when mathematical description of dynamic system is inexact.

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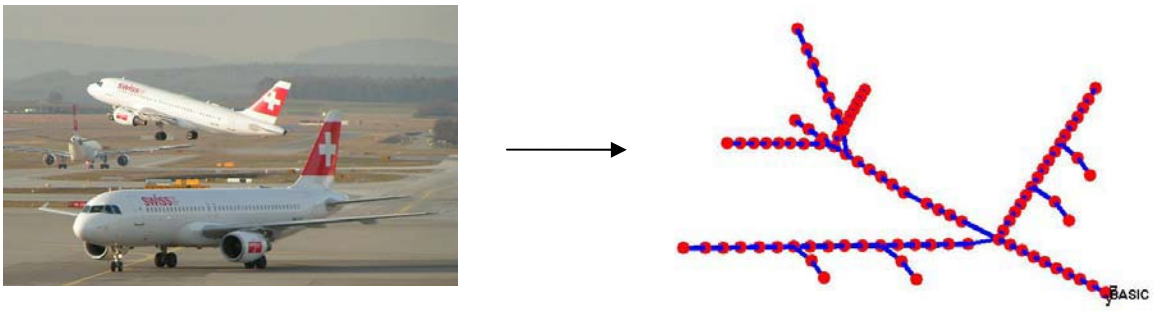
Reduced Order Models for Structural Modelling

Wolfgang Weidinger, Felix Breitenecker, Vienna Univ. of Technology, Austria
Inst. f. Analysis and Scientific Computing, Vienna University of Technology, Austria
Wiedner Hauptstrasse 8-10, 1040 Wien, Austria
Phone: +43 1 58801-11455, Fax: +43 1 58801-11499
email: wieweit@fsmat.at

When the brothers Wright did their first flights with their "Flyer" in 1903, humanity took one step forward to fulfil its dream of flying. Since this year progress was tremendous and in 1919 the first commercial aircraft - the Junkers F13 - was built. Other cornerstones like the Boeing 747 followed and this development resulted in the building of the Airbus A380 as the last and biggest achievement. In the course of this progression the methods for research and construction of these new airplanes also had to keep pace. Therefore modelling and simulation is used at an increasing rate in this industrial sector and this paper represents one of these efforts.

The aim of this work has been to enhance an existing model of an airplane, in which the number of nodes should be decreased as much as possible. This extension of the existing method aims at including element coordinate systems in the existing model. Therefore it is possible to compute bended structures which are found in the rear part of the fuselage of an airplane. Afterwards the calculated results were compared by means of modal analysis to another model which consists of substantially more nodes.

The modelling of this airplane was carried out with the help of the PSE (Program Solving Environment) MATLAB and in doing so the results of modal analysis were saved as a user-friendly .pdf-file. The number of nodes was halved successfully and the results of modal analysis remained satisfying.



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IDENTIFIABILITY OF NONLINEAR SYSTEMS: COMPUTATIONAL ASPECTS

J.Tabun[1], S. Nõmm[1], Ü. Kotta[1], C.H. Moog[2]

Corresponding author Ü. Kotta
[1]Institute of Cybernetics at TUT
Akadeemia tee 21, 12618 Tallinn, Estonia
Phone:+372 620 4153 Fax:+372 620 4151
e-mail: kotta@cc.ioc.ee

[2]Institut de Recherche en Communications et en Cybernétique de Nantes
UMR 6597 du CNRS, 1 rue de la Noë BP 92 101 - 44321
Nantes, CEDEX 03, France
Phone:+ 33 2 40 37 69 11 Fax:+ 33 2 40 37 69 30
e-mail: Claude.Moog@irccyn.ec-nantes.fr

The paper is devoted to the computational aspects of identifiability of nonlinear single-input single-output systems. Answering the question whether or not the parameters of the system can be uniquely determined from the input-output data, identifiability has a crucial importance for the quality of the identification results. There is a significant number of contributions devoted to the identifiability of nonlinear control systems. The paper [1] provides generic classification of different identifiability concepts for nonlinear continuous-time systems and [2] extends these results for the discrete-time case. In spite of the importance of the problem, in the best of our knowledge, there are just a few remarks on practical methods to verify if the nonlinear control system of interest is identifiable or not, and almost no software tools which can be used for that purpose.

The main contribution of our research is to develop practical methods for verification if a given system is identifiable in the sense of a certain identifiability concept and to implement those methods in the form of the computer algebra system *Mathematica* functions. The systems under consideration are described by their state-space equations. In [1] and [2] two main identifiability concepts are defined, *algebraic identifiability* and *algebraic identifiability with known initial conditions*. These concepts characterize the possibility to find the parameters of the system by solving a system of algebraic equations, with or without the knowledge of initial conditions. Necessary and sufficient identifiability conditions developed in [1] and [2] are stated in the language of certain subspaces of differential one forms, associated to the control system. While for some simple systems it is easy to check them directly, it is not simple task for the higher order systems or for the systems with complicated structure. Moreover, it is even more difficult to implement these conditions in the form of the software functions.

Necessary and sufficient identifiability conditions derived in this paper require mainly to compute and compare ranks of certain matrices of partial derivatives. Implementation of those conditions in CAS *Mathematica* is discussed in detail and illustrated by the examples. Additionally, the paper considers the implementation of the method to verify if the parameters of the system can be identified by the least-squares method [3].

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Alternative Groundwater Modelling

G. Höfinger, ARC Seibersdorf Research
F. Judex, TU Vienna, Austria

Corresponding Author: F. Judex
Vienna University of Technology
Wiedner Hauptstra\ss e 8 -- 10, 1040 Wien, Austria
Phone: +43 1 58801-10121, Fax: + 43 1 58801- 10199
email: efelo@osiris.tuwien.ac.at

An ever increasing human population, in turn increasing the world wide industrial output, lead to a rising demand in pure water both for human consumption and as ingredient for many industrial processes. In many regions, the surface water available does no suffice, and over the last decades more and more ground water is used.

The exploration of water bearing strata (aquifers) containing ground water bodies is a time consuming and expensive process, and especially in the industrialized countries the water bodies found are often polluted. In this case, the source of the pollution has to be established. Most often expert knowledge is used as major tool in this process, but is augmented by simulation results to test various alternatives proposed by geohydrologists. These scenarios differ in the geometric set up of the aquifer, which in turn effects the groundwater flow, and the pollution source.

Groundwater data can only be gathered via well, and if the data gathered from existing one do not suffice, new ones have to be dug. This is not only slow and expensive, but in many cases near to impossible, for example when the groundwater body is located under urban areas. As groundwater tends to flow very slowly, the time series of data should reach back very far, and the problems tend to get worse while the data for coping with them is gathered. In confined aquifers – aquifers between two impervious rock strata – this is also a massive change in the properties of the groundwater body.

Nevertheless the Finite Element Method, used for very exact computation on known geometries, is the most common tool. Most often also commercial software for groundwater simulation is based on this method, because it is well developed and can be automatized for people to use without being an expert in simulation or numerical methods [2].

Alternative methods, like cellular automata or monte-carlo[1] methods which are not as precise as the FEM method, are becoming more interesting as they tend to use more memory but less computation time. Also, their computation does not increase much with more complex geometries, because they use rules based on very small neighbourhoods. So different scenarios can be computed quite fast, with a precision based on the quality of the data.

Monte Carlo methods are most suited for the simulation spread of pollution in aquifers with known groundwater flow. The pollutant is modelled as a number of particles, which are then subjected to the convection of the groundwater flow, and diffusion, modelled by random movement. The convergence of these methods to the solution of the governing partial differential equation for a rising number of particles can be shown in some cases.

A possible use for cellular automata is the simulation of the groundwater flow itself, to get approximations for unknown groundwater streams, which in turn can be used for the Monte Carlo methods described above.

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A state space embedding approach to time discretization via an approximate normal form

J. Deutscher[1] and M. Bäuml, Universität Erlangen-Nürnberg, Germany
Lehrstuhl für Regelungstechnik, Universität Erlangen-Nürnberg
Cauerstraße 7, D–91058 Erlangen, Germany
[1]Phone: + 49 (0)9131/85-27128, Fax: + 49(0)9131/85-28715
[1]email: joachim.deutscher@rt.eei.uni-erlangen.de

This poster considers the implementation of a new approach to the time discretization of nonlinear continuous time systems. If one is interested in an sampled system of a continuous time system, then an initial value problem for a nonlinear differential equation has to be solved within the sampling interval. One approach to solve this problem is to expand the solution in a truncated Taylor series which yields a Taylor-Lie series of the sampled system (see [KK97, MNC85]). The resulting sampled system is only accurate for sufficiently small sampling periods. However, it is desirable to use large sampling periods due to the available machine time. This can be achieved by computing an approximation of the nonlinear continuous time system that admits a closed form solution of the initial value problem. The common approach is to use a linear approximation of the nonlinear system such that the initial value problem becomes linear. However in most cases the linear approximation is only valid within a limited domain.

The aim of this poster is to reveal, how the discretization of a nonlinear continuous time system presented in a companion paper (see [Deu06]) is implemented in a numerical software package. In order to enlarge the domain, where the discrete time model is valid, the nonlinear terms of the Taylor expansion are taken into account. This is achieved by calculating a nonlinear change of coordinates which transforms the terms of the Taylor expansion of the continuous time system into triangular form. In [Deu06] it is shown that the effect of the change of coordinates on the kth degree terms can be represented by a linear map between finite dimensional vector spaces. The main result of this poster is an explicit matrix representation of this linear map. The presented linear equations can be directly obtained from the Taylor expansion of the continuous time system and take the effect of the transformation in the kth step on the terms of higher degree into account. This is achieved by embedding the nonlinear system in a higher dimensional state space up to the desired degree of the terms to be transformed. In this state space of higher order the nonlinear change of coordinates becomes a linear transformation enabling the formulation of linear matrix equations. If these equations are not solvable a least square solutions is computed by using the Moore-Penrose Pseudo-Inverse. Thus, an exactly discretizable system approximation of the nonlinear continuous time system in the least square sense is obtained.

Since calculating the sampled model by integration of the triangular system may be rather tedious an alternative time discretization procedure for triangular systems is presented. In [Deu06] it is shown that every triangular system can be exactly embedded as higher order bilinear system. This step has to be evaluated using a computer algebra package. If it is not possible to calculate the solution of the initial value problem of the bilinear system with a computer algebra system a numerical procedure for computing the sampled system is proposed. Another purpose of this poster is to investigate the properties of the resulting sampled data model. To this end, expressions are derived for the coefficients of the polynomial nonlinearities of the sampled system that can be calculated. There are numerical problems which obviate a free choice of the sampling time, but even with this numerical restriction a larger sampling time can be chosen in comparison to the Taylor-Lie series representation. Two examples will illustrate the implementation procedure of the new discretization approach in a numerical software tool.

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QUASI STEADY-STATE APPROXIMATIONS IN SIGNAL TRANSDUCTION – A WORD OF CAUTION

Morten Gram Pedersen, Dept. Math., Tech. Univesity of Denmark, Kgs. Lyngby, Denmark
Alberto M. Bersani, DMMM, University "La Sapienza", Rome, Italy
Enrico Bersani, Datalink Informatica, Rome, Italy

Corresponding Author: A.M. Bersani
University "La Sapienza"
Dept. of Mathematical Methods and Models (Me.Mo.Mat.)
Via A. Scarpa 16, 00161 Rome, Italy
Phone: +39 0649766681, Fax: +39 0649766684
email: bersani@dmmm.uniroma1.it

Abstract. One of the main goals of Systems Biology is to extend the successful modeling of simple biochemical phenomena to the larger scale of intracellular signal transduction.

Enzyme reactions play a pivotal role in intra-cellular signal transduction and hence in Systems Biology. Many enzymes are known to possess Michaelis-Menten (MM) kinetics and the MM approximation, or standard quasi-steady-state approximation (sQSSA), is often used when modeling enzyme reactions, in order to simplify them. However, it is known that the MM approximation is only valid at low enzyme concentrations. This condition is usually fulfilled by experimental in vitro set-ups, but may break down in many in vivo situations. Thus, using the MM approximation with its parameter values obtained from in vitro experiments will often lead to false conclusions when simulating in vivo systems.

Recently several other mathematical approaches, such as the total quasi steady-state approximation (tQSSA), have been developed for enzymes with MM kinetics. These new approximations are valid not only whenever the MM approximation is, but moreover in a greatly extended parameter range. Hence, the tQSSA should preferably be used when simulating intracellular mechanisms, characterized by very complex interaction networks, using the usual MM parameters obtained from in vitro experiments.

We give several examples of biologically realistic scenarios where the MM approximation leads to quantitatively as well as qualitatively wrong conclusions and show that the tQSSA improves the accuracy of the simulations greatly, without the need of more advanced mathematics. In particular, we apply our considerations to the well-known MAPK cascade, which is one of the most important and most studied biochemical sub-networks, because it governs many cellular processes, such as cell proliferation and differentiation.

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A Modelica Library for System Dynamics Modelling

Günther Zauner[1], Felix Breitenecker[1], Borut Zupancic[2]
[1]Vienna Univ. of Technology, Austria; [2] Univ. Of Ljubljana, Slovenia

Corresponding Author:
Günther Zauner, Inst. f. Analysis and Scientific Computing
Vienna University of Technology, Austria
Wiedner Hauptstrasse 8-10, 1040 Wien, Austria
Phone: +43 1 58801-11455, email: Guenther.Zauner@gmx.at

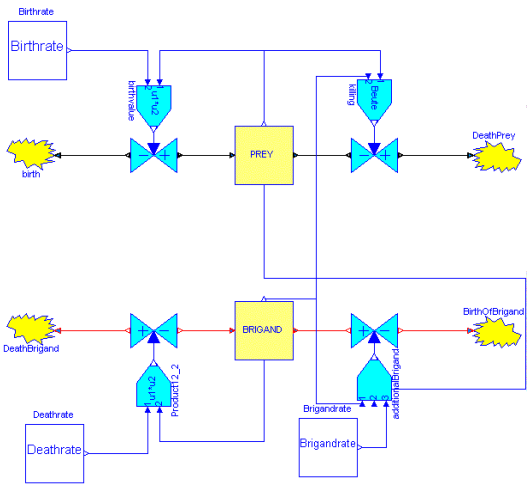
This work represents a Modelica library for System Dynamics, realized in Modelica 2.1.All standard elements were implemented referring to the definition from Jay Forrester [1]. Furthermore, it was focused on colour-coding for more user-friendliness and on implementation of units for the particular flow types, which supports the interpretation of the simulation results. As environment for the Modelica standard Dymola, a commercial surface from Dynasim, was chosen.

The library is intended to be used to model and simulate problems in socio-economic fields. The user-friendly, hierarchical structure of the designed Modelica library enables the implementation of the influence of widespread data and manifold data structures and, at the same time, clarity of the model can be maintained. Thus, it is possible to include also non-technicians directly in the process of modelling.

Modelica [2] was chosen as modelling standard because it has a more adequate structure compared to other general purpose tools like Simulink or ACSL. The elements of the designed SD library can be defined in three categories [3]:

1st group	Elements through which the flow variable is running	- Level - Source/Sink - FlowUpDown
2nd group	Rates and auxiliaries for control of the flow	- Rates - Data source - State events
3rd group	Additional components	- First order - Third order - TimeShift

Essential is a mapping of the different flow connections of System Dynamics (material, information, money, etc.) to Modelica connectors. Ten different connectors were implemented. For instance, the connector `MoneyInput` is used to define an input for money flow into a component. It is defined by the following Modelica program. Defined SD components and connections allow building up a graphical SD model (shown in figure at right). The figure also shows the different types of flows by colour-coded connection lines.




```
connector MoneyInput
   parameter Integer n=1
    "Dimension of signal vector";
     class Money = Real ( unit="Euro");
   input Money signal[n];
end MoneyInput;
```

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DYNAMICS OF AN EXPERIMENTALLY BASED CHEMOSTAT MODEL

J. Heßeler[1], J. K. Schmidt[2], U. Reichl[2,3], D. Flockerzi[3]

[1] Dpt of Mathematics and Physics, Albert-Ludwigs University, Freiburg
[2] Dpt of Chemical Engineering, Otto-von-Guericke University, Magdeburg
[3] Max Planck Institute of Dynamics of Complex Technical Systems, Magdeburg

Corresponding Autor: J. Heßeler
Dpt. of Mathematics and Physics, University Freiburg
Hermann-Herder-Str. 3, 79104 Freiburg, Germany
Phone: +49 761 203-5764, Fax: +49 761 203-5967
email: juhe@fdm.uni-freiburg.de

For microbial species competing for one limiting resource in a chemostat, mathematical models lead to the competitive exclusion principle (CEP) predicting survival of only one species in any case [1].
Quantitative data from our three-species experimental chemostat that is related to the genetic disease Cystic Fibrosis allude to coexistence of at least two competing species (Schmidt, J. K., paper in preparation).
Our project combines mathematical modeling with experimental studies, e.g. to explain this seeming contradiction between theory and experiment.

We present our extensions of the classical chemostat model complying with selected species properties of our mixed culture and achieve a characterization of these new models by use of mathematical tools from systems analysis. Furthermore we introduce our biological model system and show some of our experimental data serving as basis for the assumptions implemented into our mathematical model.
For finding possible explanations for the coexistence phenomena, one of our first aims was an investigation of the general dynamics. As a first approach we analyzed our system with two species with distinct properties.

The first assumption has a strong biological motivation: We incorporate a secondary metabolite into the classical chemostat model with Monod-type uptake functions. This secondary metabolite can be exploited as a secondary resource by one species but it also has an inhibiting effect on all species (Assumption I).
As a further assumption, we suppose interspecific competition between some species , e.g. via toxin production (Assumption II). This will change the dynamics of the system in a fundamental way. A Hopf bifurcation will occur for appropriate parameter values. Additionally and alternatively, as Assumption III, we introduce a lethal inhibitor, e.g. therapeutic antibiotics. This inhibitor is modeled in such a way that it cannot be eliminated by one of the species while being selective for the strongest competitor. This modification is very well suited for experimental validation within process engineering methodologies.
Having introduced such species specific properties of the microorganisms, we present the stability and bifurcation analysis for such extensions of the classical chemostat model. For example, the incorporation of a secondary metabolite by Assumption I is shown analytically to lead, for appropriate parameter values, to stable coexistence of competing species. Thus, the competitive exclusion principle can already be circumvented in case of the 4-dimensional chemostat variant based on Assumption I. We analyze the dynamics of the 4D and 5D chemostat models based on Assumption II and III respectively and present XPPAUT-simulations of these models for experimentally relevant parameter values (cf. [2]).
Furthermore we investigate our chemostat models with all three species that are studied in our laboratory system and discuss a more detailed modeling of the underlying resources.

This close connection between quantitative experimental data and mathematical modeling has, to our knowledge, not yet been realized for systems with more than two species and not at all for our specific experimental system of interest.

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MODELTOOL 1.0 - A MODEL TOOLBOX FOR MATLAB/SIMULINK

M. Bakošová, J. Baleja and A. Vasičkaninová, STU Bratislava, Slovakia

Corresponding Author: M. Bakošová
Slovak University of Technology, Faculty of Chemical and Food Technology, Department of Information Engineering and Process Control
Radlinského 9, 812 37 Bratislava, Slovakia
Phone: +421 2 59325353, Fax: + 421 2 52496469
email: monika.bakosova@stuba.sk

Two of the main research and teaching areas at the Department of Information Engineering and Process Control FCFT STU in Bratislava are process modelling/simulation and process control. During the years, there were created many mathematical models of various types of processes from chemical technology and various simulation environments were used for simulation. Many of models were also used for testing of various control algorithms. Nowadays, the MATLAB/Simulink is used as a simulation environment. From the variety of created models arose the necessity to develop a library of basic types of mathematical models of processes from the chemical technology. The result is the MODELTOOL 1.0 - a model toolbox for MATLAB/Simulink.

MODELTOOL 1.0 includes blocks of mathematical models of several processes: liquid holding tanks, heat exchangers, tray distillation columns and chemical reactors. All of these models are state-space models, liner or nonlinear. They are derived using mass and energy balances of modelled processes. According to the parameter setting, one block for various situations can represent various types of systems: single-input single-output system or multi-input multi-output system with specified number of inputs and outputs.

In the MODELTOOL, it is possible to find 2 models of liquid tanks – nonlinear and linearized model. Both models provide the possibility to follow the level heights in liquid tanks connected serially with or without interactions. The input variables are flow rates of inlet streams. Other optional parameters are number of tanks, valves constants, cross section areas of tanks, and interactions between tanks. The block Liquid Holding Tank – Linearized Model calculates the matrices of linear state-space description and simulates dynamical behaviour of tanks using the linear state-space model. Nowadays the MODELTOOL contains 8 blocks for heat exchangers. They represent models of serially connected flow heaters, serially connected shell heat exchangers, 3 nonlinear models of tubular heat exchangers derived under various simplifying assumptions (1 – the most simple model, 3 – the most complicated model) and 3 linear models of tubular heat exchangers derived also under various simplifying assumptions (1 – the most simple model, 3 – the most complicated model). MODELTOOL includes two models of chemical reactors. The first one is the general model for m parallel chemical reactions with n reactants. The maximum number of m is 3 and the maximum number of n is 5. The second model is the general model of the reactor with two serial reactions and one parallel reaction according to the scheme $aA \xrightarrow{k_1} bB \xrightarrow{k_2} cC$, $aA \xrightarrow{k_3} dD$. The block Tray Distillation Column allows simulation of dynamical behaviour of the tray distillation column for separation of a binary mixture. The mixture can be chosen arbitrarily as well as the number of trays and the feed tray number.

The toolbox MODELTOOL is an opened system and mathematical models of other processes from chemical technology will be gradually added to it. The using of individual blocks is simple and it does not demand special knowledge on modelling. The toolbox can be used especially for educational but also for research purposes.

Acknowledgement
The authors are pleased to acknowledge the financial support of the Scientific Grant Agency of the Slovak Republic under the grant 1/1046/04 and the financial support of the Cultural and Educational Grant Agency of the Slovak Republic under the grant No. 3/3121/05.

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FUZZY MODELLING AND IDENTIFICATION OF THE CHEMICAL TECHNOLOGICAL PROCESSES

A. Vasičkaninová and M.Bakošová, STU Bratislava, Slovakia

Corresponding Author: A. Vasičkaninová
Department of Information Engineering and Process Control, Faculty of Chemical and Food Technology,
Slovak University of Technology, Radlinského 9, 81237 Bratislava, Slovakia
e-mail: {anna.vasickaninova, monika.bakosova}@stuba.sk

Abstract. The paper deals with fuzzy identification of a chemical reactor, a system of three liquid holding tanks and a distillation column. The identification is based on measurement of input-output data. Models of the above mentioned systems were used for simulation in MATLAB/Simulink in order to obtain input-output data sequences for identification. The obtained fuzzy models are in the form of the Sugeno-Takagi neuro-fuzzy models.

1. Introduction

When dealing with the real-world systems, it is natural to consider the non-linear dynamic models of observed systems. Combination of fuzzy logic and neural networks is one of the techniques that are recently used for modelling of nonlinear and highly complex systems. In many real applications, fuzzy models can be designed on the basis of measured data.

2. Fuzzy modelling

Processes in chemical industry are in general complex, non-linear, with time-delays.
Fuzzy models can be considered as logical models, which use i*f - then* rules to establish qualitative relationships among variables in the model. Many different approaches to fuzzy identification have been proposed, see e.g. [3], [4].
Consider a chemical reactor with exothermic first-order irreversible parallel reactions. The simplified non-linear dynamic mathematical model of the reactor consists of five differential equations [1]. The measured outputs are concentrations of reactants and temperatures of reaction mixture and coolant.
A simplified mathematical model of the distillation column for separation of the binary mixture benzene and toluene derived by the mass balance of the more volatile component consists of 27 nonlinear differential equations [2]. The output variable is the concentration of the top product, the liquid flow rate inside the distillation column was chosen as the input variable.
A system of three liquid holding tanks was also modelled in MATLAB/Simulink. The output variables are levels of liquid in tanks. The input variables are flow rates of input streams.
Sugeno-Takagi neuro-fuzzy models in the form *if* x_1 *is A and* x_2 *is B then* $y=f(x)$ were supposed for the identification of three chemical processes. The fuzzy logic/neural network hybrid ANFIS structure was used to design the Sugeno-type fuzzy inference system.

3. Conclusions

Fuzzy models of the described chemical processes were designed on the basis of input-output data sequences. The Anfis structure uses a hybrid learning algorithm to identify parameters and applies a combination of the least-squares method and the backpropagation gradient descent method for training fis membership function parameters to emulate a given training data set. Data based fuzzy model can be used in the system control design and prediction.

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Parameter estimation in stochastic chemical reactions

S. Reinker[1], R. Altman[2], Jens Timmer[1]
[1] FDM, Uni Freiburg,
[2] Statistics, Simon Fraser University

Corresponding Author: Stefan Reinker
Department of Mathematics and Physics, FDM
University of Freiburg, Germany
Hermann-Herder Str. 3, 79104 Germany
Phone: +49 761 203-5828, Fax: + 43 1 58801- 10199
email: reinker@physik.uni-freiburg.de

Gene regulatory, signal transduction, and metabolic networks are major areas of interest in the newly emerging field of systems biology [1]. In living cells, stochastic dynamics play an important role because of small molecule counts, e.g. of RNA, and are believed to be the source of most intracellular noise. The latest experimental imaging techniques enable researchers to measure biochemical processes at the molecular level inside living cells, such as small molecule counts of reactants. In systems with only a few molecules, classic mass action kinetics are no longer valid for describing the reaction dynamics. Therefore the usual approach to estimating reaction rates by fitting solutions of law of mass action differential equations to reactant concentrations is not appropriate.

In this work, we consider the problem of estimating stochastic reaction constants from molecule count data measured, with error, at discrete time points. For modeling the system we use a hidden Markov process in the Gillespie framework of stochastic reaction system [2]. Because of observation error or incomplete measurements, the true molecule counts are hidden states. Transitions between states correspond to reaction events when molecules collide. The state transition probabilities can be expressed in terms of collision probablities based on the numbers of molecules and reaction propensities. Thus the transitions of the Markov process are state dependent and change in time.

Little work has been done on the inverse problem of parameter identification [3] in stochastic reaction systems. Here, we propose two different algorithms for estimating the unknown model parameters. The first is an approximate maximum likelihood method which searches the state space of possible reaction paths. Approximations necessary for computational simplicity and speed include a maximum cap of possible reactions in a sampling interval and limited observation errors. Using an optimization method to maximize the likelihood of the data, this method gives good estimates of the reaction parameters in systems with few possible reactions in each sampling interval.

Our second algorithm treats the data as exact measurements and approximates the number of reactions in each sampling interval by solving a simple linear equation with a singular value decomposition method. Maximum likelihood parameter estimates based on these approximations provide good results even in complex reaction systems with many thousands of molecules.

The parameter estimation performance of these two algorithms is demonstrated on simulated data in a simple two molecule reaction system as well as the more complex Lotka system which exhibits stochastic oscillations. We analyze the effects of sampling rate and observational noise on identifiability and algorithm performance, and calculate confidence bounds of parameter estimates.

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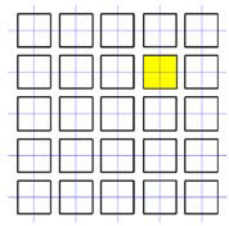
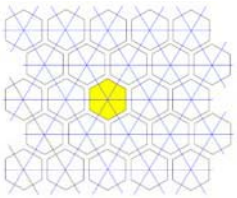
Classical ODE Modelling versus Cellular Automata Modelling of a SIR-type Epidemic

Nikolas Popper[1], Harald Hötzendorfer[2], Daniel Leitner[2], Felix Breitenecker[2]
[1]Drahtwarenhandlung – Simulation Services, Vienna, [2]Vienna Univ. of Technology, Vienna

Corresponding Author:
Nikolas Popper, Drahtwarenhandlung – Simulation Services
Neustiftgasse 57-59, Vienna, Austria
email: Niki.Popper@Drahtwarenhandlung.at

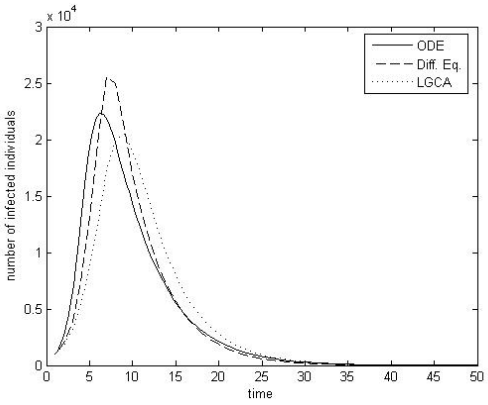
This contribution compares different modelling approaches for a SIR-type epidemic and presents experiments with these models. First, the classical ODE model found in literature is presented. After a short introduction into cellular automata the dynamics of a SIR-type epidemic is modelled by a lattice gas cellular automaton model (LGCA model), which involves dynamic propagation in time and space. Furthermore, based on the average states of the LGCA model, a difference equation model (DifferenceE model) can be derived, which is similar to the ODE model.
Experiments with these models show similarities of results, "convergence" of the LCGA model to the ODE model, and spatial and temporal behaviour of different vaccination strategies using the LCGA model.
For joint model implementation and simulation of ODE model, LGCA model and DifferenceE model features of simulations systems are discussed shortly. Results are presented with a MATLAB implementation. The investigated models are also used in ARGESIM comparison "*Temporal and Spatial Evolution of a SIR-type Epidemic*"





LGCA Model for SIR-type Epidemic. The spread und recovery of an infection can be interpreted as a diffusion process among particles (= peoples). Therefore, a lattice gas cellular automaton (LGCA) can be considered to describe the epidemic. LGCA are two-dimensional cellular automata with particles moving from cell to cell during each time-step of the automaton. Therefore, the definition of different states for the cells becomes obsolete, rather each particle can hold different states (in our case this will be susceptible, infected or recovered). Neighbourhood now refers to all particles in one cell and not to the surrounding cells.
Since LGCA descend from fluid dynamics, basic physical quantities like mass and momentum are conserved. Evolution (the motion of the particles) consists of propagation and collision. We have to distinguish between the HPP (Hardy, de Pazzis, Pomeau - 1973) and the FHP (Frisch, Hasslacher, Pomeau - 1986) model. The first one is composed of a square lattice which contains no more than four particles per cell (see figure at right).

Convergence of LCGA to ODE model. In the LCGA model, spatial grouping of infected individuals can be observed which will consequently change the results of the simulation in comparison with the continuous approach. For lattice Boltzmann cellular automata it can be shown, that the averaging states converge under certain circumstances to solution of the continuous Boltzmann equation. For the investigated LGCAs, a kind of "convergence" can be shown experimentally. The idea is to prevent from clustering in the LCGA and observe again the average states.
For these purpose, one must ensure perfectly uniform distributions for all three groups of populations by randomly rearranging all individuals in every time step of the automaton. Avoiding inhomogeneities by rearranging all individuals after every time step of the automaton results in fairly similar behaviour for the system of ODEs, the difference equations and the FHP-LGCA (figure at right).



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Electrical stimulation of a human thigh with conductive implant: a finite element study

F. Dohnal, F. Rattay and M. Reichel, TU Vienna and Med.Univ., Vienna, Austria

Corresponding Author: F. Rattay,
Vienna University of Technology
Wiedner Hauptstraße 8 - 10, 1040 Vienna, Austria
Phone: +43 1 58801-10114, Fax: + 43 1 58801- 10199
email: rattay@tuwien.ac.at

Electrical stimulation have been developed for reactivating and building up muscle fibres, either with surface or implanted electrodes. The surface systems are non-invasive, since no surgery is required. However, they require accurate electrode placement and extremely high currents in order to overcome the skin-fat layer. The implanted electrodes offer higher selectivity and can reach deeper muscles not accessible from the surfaces.

The stationary potential distributions and the resulting capability of activating denervated skeletal muscles for different electrode arrangements are calculated with the MATLAB-based finite element program FEMLAB. Two models of the human thigh are considered using isotropic and anisotropic layers with averaged values of conductivities. The electrodes are located outside the human thigh, on the skin, or inside the human thigh, on or inside the bone. A three-dimensional model is investigated respecting the influence of the part outside the symmetry plane. Systematic case studies are performed in order to compare the benefits and the drawbacks of each electrode assembly.

The human thigh is modelled by four axial-symmetric layers, to which we particularly assign isotropic or anisotropic conductivities: the skin-fat layer, the muscle layer, the bone layer and the conductive implant layer. Additionally, we respect the necessary and highly conductive bolts of the conductive implant, that directly connects the muscle layer with the otherwise isolated implant. The amount of charge necessary for excitation can be determined directly by integration. Minimizing charge, by using the most beneficial electrode arrangement for a specific purpose, is an important consideration for safety reasons by minimizing power consumption. The electrodes are provided by a constant potential. The comparison is carried out by determining surfaces of equipotential inside the whole thigh, the necessary current that have to be provided to the electrodes to ensure their constant potential and the resultant activating function along certain muscle fibres. An exemplary plot of surfaces of equipotential for the arrangement of an electrode on the skin and using the implant inside the bone with its highly conductive bolts as the second electrode is shown in Fig. 1. The four axial symmetric layers are indicated by thick-lined wireframes.

The following steps are necessary for the performance of this comparison: building a simplified model of a human thigh in MATLAB/FEMLAB, calculation of the voltage potential inside the thigh using FEMLAB, and finally, export into and further processing of these voltage potentials in MATLAB for determining of lines of equal potential in a defined cross-section of the thigh and determining of potential curves and their first and second directional derivatives along prescribed muscle fibres, determining the activating function. An automated MATLAB-procedure is developed that is capable to evaluate the tasks above. Defining the main dimensions of the geometry of the human thigh, three-dimensional FEMLAB-objects are generated, the boundary constraints are set automatically in dependency of the chosen electrode arrangement and the averaged conductivities are assigned to the different layers. After meshing, the problem is solved iteratively. This procedure can be used as a comfortable tool for testing the sensitivity of the model.

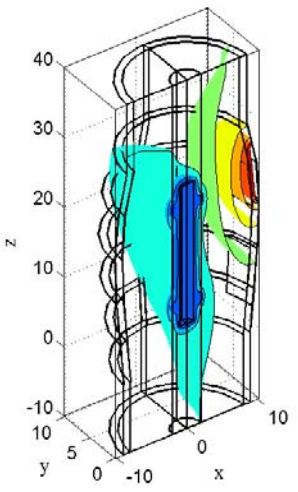

Figure 1 Surfaces of equi-potential inside the thigh for one electrode on the skin and one inside the bone; lengths in cm.

Nerve fibres lying at different distances from the electrode feel different potential distributions. Muscle fibres lying deep inside the thigh are hard to stimulate by electrodes lying on the skin. In this case the necessary current to exceed the activation threshold of the muscle fibres is relatively high, and the underlying tissue may be damaged by the electrode. For this purpose a different electrode arrangement with at least one implanted electrode is more accurate.

This investigation helps to test electrode configurations concerning lower stimulation currents and better spatial selectivity of stimulation.

MATHEMATICAL MODELLING OF AN AUTONOMOUS VEHICLE FOR NAVIGATION CONTROL

K. Moriwaki and K. Tanaka

The University of Shiga Prefecture
2500 Hassaka-cho, Hikone, Shiga 522-8533, Japan
E-mail: {moriwaki, k-tanaka}@mech.usp.ac.jp

Abstract. The problem of modelling and control for autonomous vehicles is considered. Mutual interactions among vehicle motion dynamics are evaluated. It is proposed the mathematical model suitable for describing and simulating the whole motion of autonomous passenger vehicles.

1. Modelling of an Autonomous Vehicle

The passenger vehicles are evaluated from many points of views, such as riding comfort, vehicle position, stability, manipulability and so on(Figure 1). The performance of vehicle control in technically is seperated into several control items and considered to each item independently. The mathematical model for steering control of an autonomous vehicle has usually two degrees of freedom, which consider the lateral motion and the yawing motion[1],[2]. The model for suspension dynamics, which is deeply related to riding comfort, has also two degrees of freedom, which consider the bouncing motion and the pitching motion[3],[4]. The above mentioned models are not enough to treat the problem of total motion control for autonomous vehicles. The specifications of tires must also be considered in the whole motion control of vehicles and they have strong nonlinearity[5]. There are, furthermore, mutual interactions among them, which are inevitably considered in the problem of the whole motion control for autonomous passenger vehicles(Figure 2).

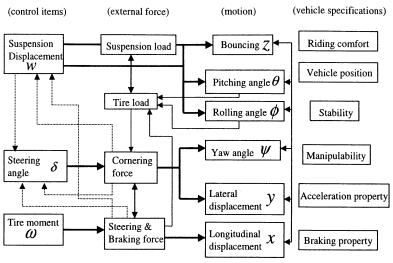

Figure 1: Vehicle control items and mutual interactions

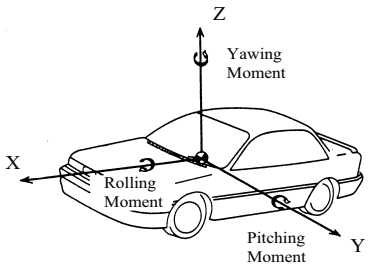

Figure 2: Rigid-body model of four wheel vehicles

2. Motion Control of an Autonomous Vehicle

Objectives of steering control and suspension control are to achieve tracking the prescribed route to a destination[6] and stabilizing the rolling motion and pitching motion of a vehicle during moving, respectively. These problems are formulated in the form of nonlinear H_∞ control. Hamilton - Jacobi equations are obtained to solve and/or simulate numerically.

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COURNOT MODEL WITH UNKNOWN COSTS

Sofia Barros, Fernanda Ferreira, Flávio Ferreira and Alberto Pinto, FCUP and ESEIG/IPP, Porto, Portugal

Corresponding Author: Fernanda Ferreira
ESEIG/Instituto Politécnico do Porto
R. D. Sancho I, 981, 4480-876 Vila do Conde, Portugal
Phone: +351 252 291700, Fax: +351 252 291714
email: fernandaamelia@eseig.ipp.pt

A game is a situation with any kind of interactions, and it has, by definition, participants who are called players. A player may be interpreted as an individual or as an organization making a "racional" decision. The players receive payoffs that depend on the combination of decisions just taken. There are games of complete information, in which the players' payoff functions are common knowledge and games of incomplete information (also called Bayesian games), in which at least one player is uncertain about another player's payoff function. In the first case, the usual solution concept is the Nash equilibrium: a decision combination is a Nash equilibrium when, if one player sticks rigidly to his decision in the combination, then the other player cannot increase his reward by selecting other than his decision in that combination. That is, each player's strategy must be a best response to the other player's strategies. A Nash equilibrium in a Bayesian game is called a Bayesian Nash equilibrium. The case that we will study belongs to the class of Bayesian games, since there are market conflicts in which each firm knows its production costs, but does not know the production costs of the other firm. Let E_1 and E_2 be two firms, sole producers of a homogeneous product. The firms simultaneously choose output levels, respectively, $q_1 > 0$ and $q_2 > 0$, with the purpose to maximize its expected payoff. We suppose that the inverse demand function is decreasing and linear in an interval $[0, a/b]$, with $a, b > 0$. More precisely, let

$$P(Q) = \begin{cases} a - bQ, & \text{if } Q < a/b \\ 0, & \text{if } Q \geq a/b \end{cases}$$

be the inverse demand function, where $Q = q_1 + q_2$ is the aggregate quantity.

We consider an economic model in which we suppose that each firm has two different technologies, and chooses one of them following a probability distribution. The utilization of one or the other technology affects the unitary production cost. The following probability distributions of unitary production costs are common knowledge:

$$C_1(q_1) = \begin{cases} c_A q_1, \text{ with probability } \phi \\ c_B q_1, \text{ with probability 1-}\phi \end{cases}, \qquad C_2(q_2) = \begin{cases} c_H q_2, \text{ with probability } \theta \\ c_L q_2, \text{ with probability 1-}\theta \end{cases}.$$

We suppose that $c_A > c_B$, $c_H > c_L$ and $c_A, c_B, c_H, c_L < a$. Moreover, we suppose that the highest unitary production cost of any firm is greater than the lowest unitary production cost of the other one, that is, $c_A > c_L$ and $c_H > c_B$. Otherwise, the conclusions will be obviously.

Firm E_i' payoff is given by

$$\pi_i\left(q_i(c_i), q_j(c_j)\right) = q_i(c_i)\left(a - b\left(q_i(c_i) + q_j(c_j)\right) - c_i\right),$$

where c_i is the firm E_i's unitary production cost, for $i, j \in \{1,2\}$ and $i \neq j$.

After determine the quantities in the Bayesian Nash equilibrium, we conclude that, for each firm, the best payoff occurs in the case of complete information, and when the firm uses its cheapest technology and the other firm uses its most expensive one. For the consumers, the best (lower price) occurs in the case of complete information, and when both firms use their cheapest technologies. Under the point of view of scanty natural resources, the "best situation" corresponds to the case of complete information, and both firms use their most expansive technologies.

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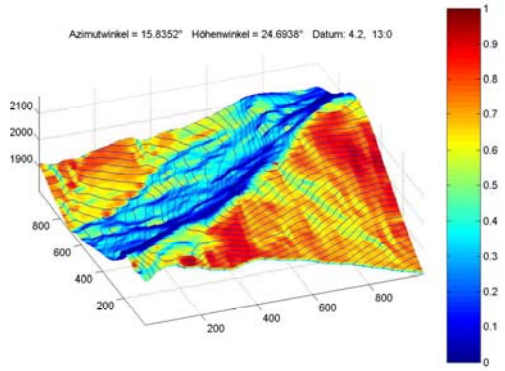
TWO-DIMENSIONAL SNOW TEMPERATURE SIMULATION

Harald Teufelsbauer, TU Wien & BOKU Wien, Austria

Vienna University of Technology
Wiedner Hauptstraße 8-10, 1040 Wien, Austria
email: harald.teufelsbauer@gmx.net

For studying the processes which are going on in the snow cover, the change of snowtemperature is very interesting. Different temperature gradients cause different metamorphoses of the snow grains within the snow cover. Therefore a precise calculation of the temperature is a necessary basis for further research.

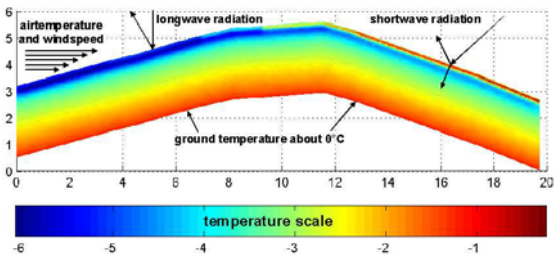
There are already existing models to calculate snow temperatures, but these models are just one-dimensional. The current research works on the enlargement of the one-dimensional models to two dimensions. This has the advantage that a whole section of a slope can be simulated and thus, the information someone can get about the snow cover is not just the view on a single point but a flexible calculation of different slopes and directions. The two-dimensional calculation makes the process of modeling more difficult. Data for simulation are measured with automatic measure stations. These stations log all input and evaluation data for the simulation.



To calculate a one-dimensional temperature profile direct at the measurement station, data which are logged by the station can be used for simulation. One of the improvements of two-dimensional simulation is the conversion of the measured data to other expositions and slopes. This should make it possible to simulate the snow temperature on inaccessible areas of the mountains. Therefore it is essential to calculate the relative sun intensity and possible shadows caused by other mountains for each section point of the simulation area.
In the left figure the dark red areas the sunrays impinge in the angle of 90° and the dark blue areas are shadowed. That effects that the measured solar radiation at the automatic measure stations can be converted to any point in the area. Due to the reason that solar radiation is one of the most important energy source it influences the temperature of the snow cover very high. Other parameters which are very important for the energy flux between atmosphere and snow cover are wind speed, air temperature and longwave radiation which is sent out from every object. It is important to explore all energy fluxes which influence the snow cover to find suitable boundary conditions for solving the heat equation.

$$\rho(x,y,t) \cdot C_{eff} \cdot \frac{\partial T}{\partial t} = \nabla \cdot (k_{eff}(\rho)\, \nabla T) + f(x,y,t)$$

The *neuman boundary condition* describes the energy flux through the snow surface and $f(x,y,t)$ is the source term following the *Law of Lambert-Beer*, which represents the heating within the snowpack, caused by the shortwave radiation. Solving the heat equation with a two-dimensional finite element method, leads to a two-dimensional heat distribution. The plot on the right side shows the different temperatures of the snow cover caused by different energy fluxes between south and north exposition and different slopes.



Modeling of Fire Protective Materials

C. Trenado, D. J. Strauss, B. Reinhard and A. Alther, INM Saarbrücken, Germany,
T. Smuc and A. Maksimovic, Rudjer Boskovic Institute Zagreb, Croatia.

Corresponding Author: C. Trenado
Leibniz-Institute for New Materials
Im Stadtwald, Building D2.2, 66123 Saabrücken, Germany
Phone:+49-681-9300-155, Fax: +49-681-9300-242
email: trenado@inm-gmbh.de

Abstract

Fire retardant intumescent materials start to bubble in response to fire and swell into a robust foam. They provide protective coatings through absorption of heat by endo-thermic reactions and through insulating properties of the final structure. Recently, aqueous intumescent nanocomposites based on nanoscaled SiO2 particles have been introduced by the Institute for New Materials and may lead to a significant improvement of general fire protective system.
A reliable mathematical model representing the heat flow characteristics of these materials does not exist up to now, but it is indispensable for an optimization of fire retardant systems containing this composite. Moreover, such a model might provide a deeper understanding of the mechanisms determining the excellent thermal insulating properties of the composite and may thus help to derive optimization objectives. In this study, we present the first macroscale heat flow model of this nanocomposite.
Our model represents the phase change from a virgin material (the gel) to a porous material (the final structure with bubble inclusions and after the carbonization of the organic compounds) by a moving mushy front, mainly driven by outgassing.
Here we do not consider a (hard) Heavyside phase front, usually used in problems of the Stefan type, which is more natural from a physical point of view. For this, a generalized form of the transient heat equation with a drain term representing the absorption of heat by endothermic reactions is employed. An additional mass conservation equation is coupled to this heat equation using a temperature dependent empirical function $\Psi(T)$ for the mass loss due to outgassing.
This mass conservation equation is also used to derive the change of the porosity (normalized inverse of the density ρ_n) of the material and the effective dynamic thermal conductivity (according to the Maxwell model). The dynamic porosity is related to the averaged bubble growth and growth limits are introduced, taking the stability of the bubbles into account. The stability of bubbles has shown strong evidence to be related to the insulating properties of the porous phase.
The equations were solved in a domain Ω using the finite element method. Our model provided a high correlation to the oven measurements using 1D and 2D numerical simulations. In particular, our model allowed for a representation of the temperature gradients in space over time and exhibited a good qualitative correlation in the phase change behavior, which was analyzed in a different set of experiments such as thermo-gravimetric analysis.

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MULTISCALE SIMULATION OF HUMAN BLOOD FLOW IN ARTERIES

Johannes Kropf and Siegfried Wassertheurer

Corresponding Author: J. Kropf
ARC Seibersdorf research GmbH, Div. Biomedical Engineering, A-2444 Seibersdorf
email: johannes.kropf@arcsmed.at

Abstract. A multiscale model for simulation of the human cardiovascular system has been developed. The model combines linear and non-linear approaches, as well as lumped parameter models. In detail, for simulation of the arterial tree a linearised model based on the Womersley solution is used to computed boundary data and impedances, while the problem itself is solved numerically by computing the one-dimensional Navier-Stokes equations for flow in elastic tubes. Other parts of the system which are of fewer interest are solved by usage of lumped parameter models. Furthermore, parameters are identified by measured data after backward computation and different models for the boundary values are used.

Introduction

In the last four decades several mathematical models have been developed to simulate the behaviour of the cardiovascular system (CVS). The range starts from simple lumped parameter models and ends in 3-dimensional finite elements model for the arterial tree. To satisfy the needs of being able to identify and adaptable to measured data, our model uses amenity of different models. Parts of higher interest are modeled more detailed whereby other parts are modeled as simple as possible.

Model Description

The parts which are not important for our considerations are modeled by simple lumped parameter models, which have the advantage that few physiological parameters have to be identified. The part of interest is the arterial tree which is modeled with a linearisation of the Navier-Stokes equations.
A special focus is on models for termination segments of the vascular bed. During development of the all in one model it became obvious that this is a key task because this data cannot be identified directly by measurement and so other methods became necessary.
All of them are combined to a comprehensive model considering the behaviour of the whole system.

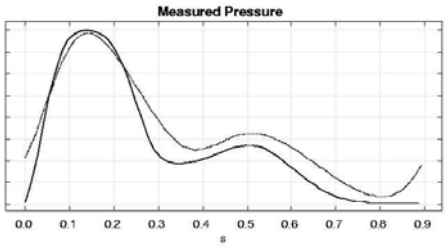

Figure 1: measured and computed blood pressure in the a. femoralis

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MEASURING PROCESS CAPABILITY INDICES

K. Rezaie, B. Ostadi, M. R. Taghizadeh
Corresponding Author: K. Rezaie
University of Tehran
Department of Industrial Engineering, Faculty of Engineering, University of Tehran,
Phone: +98 21 88021067, Fax: +98 21 88013102
email: krezaie@ut.ac.ir

Process capability indices, C_p and C_{pk} have been proposed in the manufacturing industry and the service industry providing numerical measures on whether a process is capable of reproducing items within the specification limits preset in the factory. In recent years an increasing number of organizations use process capability studies on a regular basis. Contemporaneous with the increasing number of organizations using process capability studies, warnings have been launched that imprudent use of numerical measures of capability, the so-called process capability indices, might lead the user to make erroneous decisions. In this paper, the process capability indices are presented and process capability studies be presented from a practical point of view.

PROCESS CAPABILITY AND PROCESS PERFORMANCE

K. Rezaie, M. Rabbani, M. R. Taghizadeh, B. Ostadi
Corresponding Author: K. Rezaie
University of Tehran
Department of Industrial Engineering, Faculty of Engineering, University of Tehran,
Phone: +98 21 88021067, Fax: +98 21 88013102
email: krezaie@ut.ac.ir

Once a process is in statistical control, that is producing consistently, you probably then want to determine if it is capable, that is meeting specification limits and producing “good” parts. Process capability indices are useful for assessing the capability of manufacturing processes. In this paper, the process capability indices and their estimators are presented and related to process parameters. Also, the capability indices have interpreted and steps in determining process capability have presented. Finally, process performance indices are presented.

Modelling the Human Blood Glucose Regulation – A MATLAB GUI for Comparing Models

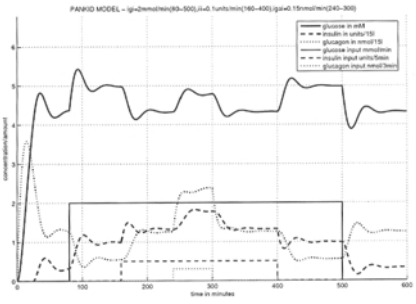
Andreas Ernst[1], Juliane Höbarth[2], Felix Breitenecker[2]
[1]ARCS Biomedical Engineering, [2]Vienna Univ. of Technology, Vienna; Austria

Corresponding Author:
Andreas Ernst, ARCS Biomedical Engineering, Floragasse 7, 1040 Vienna, Austria
email: efelo@fsmat.at

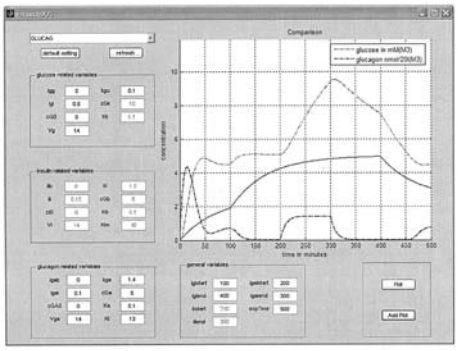
In the course of [2] a software, more exactly a MATLAB GUI, for comparing and analysing different models for the blood glucose regulation was developed. In this work the models were also analysed for the properties of observability, controllability and stability, but we will not go into these details here. The human body gets his energy from glucose (= sugar) which is extracted from carbohydrates. Hence the time of ingestion (= input of carbohydrates) and the time the glucose is needed is not the same and thus there are mechanisms in the body that can save glucose and also keep the glucose level in the blood constant. The storage of the energy (in liver, muscles and fat) can only happen when the glucose is transformed in glycogen. For this transformation the hormone insulin, which is produced in the pancreas, is needed. The antagonist of insulin is glucagon. It is also produced in the pancreas and is secreted when the glucose concentration in the blood falls under a certain level.

The model **GLUCID**. This is a simple first order model for the blood glucose regulation by the kidney. All other system components involved in blood glucose regulation remain neglected. Te disease juvenile diabetes mellitus (type I diabetes) justifies the design of a model based on blood glucose regulation by the kidney alone. In this type of diabetes the endocrine pancreas does no longer produce insulin. Dangerously high blood glucose concentrations may occur, which can only be removed from the blood by the kidneys over the urine.

The model **INSUL**. In the model INSUL the blood glucose regulation is modelled only through the hormone insulin. It is a one-compartment model with an additional feedback loop. The compartment contains two substances, insulin and glucose. This results in a second order model with two states.
In this model it is also possible, by setting parameters, to simulate juvenile diabetes where the pancreas is unable to produce insulin.



The model **PANKID** is the most complex model for blood glucose regulation discussed in [2]. It is a combination of the known models and represents the blood glucose regulation in the human body by the kidney, the hormone insulin and the hormone glucagon. The whole process of blood glucose regulation is extremely complex and even this model is a strong simplification. This model contains three state variables, the concentration of glucose, insulin and glucagon. The model is described through three first order linear ordinary differential equations – one for each substance.
The system analysis gives that the model is controllable and observable in all settings. All occurring parameters are due to physiological reasons ≥ 0 and thus it is possible to show that the system is asymptotically stable. In this model is it also possible, by setting the right parameters, to simulate several diseases like juvenile diabetes mellitus, liver diseases where the liver does not respond to glucagons in providing the blood with glucose or special types of tumours that secrete insulin constantly.



The **GUI**. In the pull down menu you can select one of the implemented models for glucose regulation. According to the model one have chosen it is now possible to enter values in the appropriate variable fields. If one is not yet experienced with the right parameter settings of the models, one can push the button "default setting" to obtain values to simulate a healthy person's blood glucose regulation. With setting the right parameter values it is now also possible to simulate the diseases mentioned above. It is possible to either plot a graph with new settings in an empty plotting or by using the "Add Plot" Button to plot a graph with different settings in the same window. So it is possible to compare the different models directly.

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