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Abstract Volume

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Proceedings
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Volume 1: Abstract Volume

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Preface

The possibility to solve certain problems and the quality of a solution obtained for a specific task depend essentially on appropriate modelling of the task in question. In many fields of application this leads to the necessity to model the dynamic and static properties of a system to be constructed, to be improved or to be influenced, but also all relevant background information connected with this task such as restrictions on controls or states, wanted and/or unwanted smoothness properties of solutions and many others. Normally, it will not be possible to describe all details of a system's behavior or all requests imposed on the solution by traditional mathematical expressions which are at the same time an accurate description of the task and sufficiently easy to handle. This is only in part due to the fact that normally not all information is available at all or at acceptable cost but also due to the fact that quite often requests can be formulated rather vaguely or, because the model of the respective task resulting from a rather accurate description would be of a size or of a complexity which can not be handled by men and/or computers. Hence, it is always the decision of the modeler what is to be included in the model and whether a model of the complete task is to be created or e.g 'only' a model of the dynamic behavior of the system to be investigated or to be influenced.

Moreover, in some cases, the system under investigation and its behavior are understood rather well. In such cases an appropriate model of the system's behavior will assist in finding a good solution of the problem to be solved. In other situations a model of the system's behavior is primarily intended to help for a better understanding of what is going on in the system. Examples for the first case are many types of design problems connected typically with engineering systems, such as controller design, design of a production line etc. whereas the request for an improved understanding is often found in connections with non-engineering systems such as biological or medical systems, economic or environmental systems and their control etc.

There is a rather wide consensus that mathematical modelling i. e. abstraction and formalization, is of intrinsic importance. Moreover, most engineers and scientists know quite well that appropriate modelling is far from being easy and that the quality of a design depends strongly on the quality of the model. One of the most important challenges connected with proper modelling is the request to model indeed the given task i. e. all relevant information, restrictions, demands, goals etc. In control engineering not only a model of the plant and constraints on relevant physical variables must be put in a mathematical form but also other requests such as that the resulting mathematical control law must allow for implementation by means of a certain type of equipment etc.

By now, considerations such as these are accepted in general and especially by those involved in the solution of problems by using computers what means by using – directly or indirectly – mathematical methods, no matter whether these persons work at a scientific institution or in an industrial environment.

However, the area of application determines to a certain extent the knowledge of basic modelling principles, preferences for modelling approaches, for certain methods for model simplification and order reduction or, for parameter estimation etc. Moreover, many things are discovered repeatedly. Therefore, a conference on mathematical modelling has not only the aim to present new methods, successfully used ideas, and new modelling principles applied in certain concrete applications but it also the aim to bring together scientists working in theory and in many areas of applictions and thus, to allow for a fruitful and stimulating exchange of ideas.

Consequently, the 4th International IMACS Symposium on Mathematical Modelling (4th MATHMOD) is devoted to the mathematical (or formal) modelling of all type of systems no matter whether the system is

* dynamic or static
* deterministic or stochastic
* continuous or discrete or hybrid
* lumped parameter or distributed parameter
* linear or nonlinear
* or of any other nature.

Thus, a wide variety of formal models is to be discussed and the term mathematical modelïncludes 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 invited papers, of contributed papers and of posters. Volume 2, the Full Papers' Volume, at 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. The first survey to be presented is concerned with multidomain or 'multiphysics' systems and their control systems which have to be designed as integrated systems. Background and tools for a port-based approach to integrated modelling and simulation are discussed in general and in view of mechatronic systems which are a widely discussed and important class of such multidomain systems.

The second plenary talk is concerned with the modelling of snow mechanics and avalanche dynamics, as an example of a complex system for which validation seems to be restricted because of the lack of observations with sufficient quality. At a first glance, this topic seems rather special and of interest primarily for a small group of scientists. Yet, it is a good example for the importance of interdisciplinary discussions: Possibilities and problems of various modelling approaches are discussed by giving avalanche prediction and avalanche dynamics. Further, observations and simulations with the FE-method show the high influence of the boundary conditions (roughness) which gives a clear hint how to improve the modelling concept in the future.

The third survey is again concerned with rather complex system and its modelling for control. Controller design is also a topic of this talk. The task is again a multi-disciplinary one, controller design has to account for the trade-off between economy and emission improvement what can be successfully accomplished by using fuzzy concepts.

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 our colleague F. Urbanek and the ARGESIM team for their support in the preparation of these Proceedings.

Vienna, January 2003 I.Troch, F. Breitenecker

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Plenary Lectures

PORT-BASED MODELING OF MECHATRONIC SYSTEMS

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Many engineering activities, including mechatronic design, require that a multidomain or 'multi-physics' system and its control system be designed as an integrated system. This contribution discusses the background and tools for a port-based approach to integrated modeling and simulation of physical systems and their controllers, with parameters that are directly related to the real-world system, thus improving insight and direct feedback on modeling decisions.
The main focus of this contribution is on the generic problem context of the dynamic (i.e. 'changing in time') behavior of systems that belong to the area of the engineer and the mechatronic engineer in particular. These systems can be roughly characterized as systems that consist for a large part of subsystems for which it is relevant to the dynamic behavior that they obey the basic principles of macroscopic physics, like the conservation laws and the positive-entropy-production principle. The other part consists of submodels for which the energy bookkeeping is generally not considered relevant for the dynamic behavior. Such parts are generally addressed as the signal processing part ('controller') that is commonly for a large part realized in digital form. This contribution deals particularly on the description of the part for which energy bookkeeping is relevant for the dynamic behavior, while keeping a more than open eye for the connection to the signal part, either in digital or in analogue form.
It is argued that port-based modeling is ideally suited for the description of the energic part of a multidomain, sometimes also called multi-physics, system or subsystem. This means that the approach by definition deals with mechatronic systems and even beyond those.
Port-based physical system modeling aims at providing insight, not only in the behavior of systems that an engineer working on multidisciplinary problems wishes to design, build, troubleshoot or modify, but also in the behavior of the environment of that system. A key aspect of the physical world around us is that 'nature knows no domains'. In other words, all boundaries between disciplines are man-made, but highly influence the way humans interact with their environment. This is why a domain-independent representation to represent a port-based approach, viz. bond graphs, will be introduced to represent the ideas behind port-based modeling. The examples will use a tool that is based on this approach, viz. 20-sim (www.20sim.com).
Several attempts to unified or systematic approaches of modeling have been launched in the past. In the upcoming era of the large-scale application of the steam engine, the optimization of this multi-domain device (thermal, pneumatic, mechanical translation, mechanical rotation, mechanical controls, etc.) created the need for the first attempt to a systems approach. This need for such a 'mechathermics' approach was then named thermodynamics. Although many will not recognize a modern treatment of thermodynamics as the first systems theory, it certainly was aimed originally in trying to describe the behavior of such a system independently of the involved domains. Its basic concepts, energy and, to some extent, entropy, also form the basis of the port-based approach to modeling.
Obviously, a smooth connection is needed between the information-theoretical descriptions of the behavior of digital systems and physical systems theory. Since their introduction bond graphs have allowed the use of signal ports, both in- and output, and a corresponding mix with block diagrams. As block diagrams can successfully represent all digital operations similar to mathematical operations, the common bond graph/block diagram representation is applicable. This graphical view supports a hierarchical organization of a model, supporting reusability of its parts.
The port-based approach may be considered a kind of object-oriented approach to modeling: each object is determined by constitutive relations at the one hand and its interface, being the power and signal ports to and from the outside world, at the other hand. Other realizations of an object may contain different or more detailed descriptions, but as long as the interface (number and type of ports) is identical, they can be exchanged in a straightforward manner. This allows top-down modeling as well as bottom-up modeling.
This contribution is concluded with an example that demonstrates how a port-based approach to modeling enhances insight via immediate feedback on modeling and conceptual design decisions.

MODELLING AND SIMULATION IN SNOW SCIENCE

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Modelling of complex systems or complex behaviour (Prigogine et al., 1990) is obviously not trivial. Natural processes with which we deal in snow mechanics and avalanche dynamics possess many features which complicate the description of both the whole system under concern as well as single events. The fact that worldwide more then hundred avalanche models are used to calculate the run-out can be interpreted in two ways: First, it seems to be difficult to find a best fit modelling concept to describe the process and second, the validation process seems to be restricted because of the lack of observations with sufficient quality. But modelling and simulation of real world phenomena with the aim to support quantitative risk analysis can only deliver satisfying reliability, if the models depict reality with all relevant influence parameters and subsystems.

It is the inherent quality of abstraction to reduce complexity. But there is no pure logical-analytical method how to perform this reduction in order to achieve a simplified image of reality with high generality. Numerous publications appeared in the last decade to this topic, which try to handle the problem from different points of view (e.g. M. Gellman 2000, I. Prigogine 1999, R. Riedl 2000, G. Fasching 1989, G. Woo 1999). In order to disrobe this claim for deriving proper subsystems from superficiality examples in the field of snow mechanics, avalanche prediction and avalanche dynamics are given in order to show the possibilities and problems of various modelling approaches.

Snow mechanics: Snow mechanical investigations are often concentrating on the strength of the snow cover itself in order to describe the mechanical behaviour. But observations and simulations with the FE-method show the high influence of the boundary conditions (roughness) which gives a clear hint how to improve the modelling concept in the future.

Avalanche release probability: The comparison of classical statistical models, self learning algorithms and a physically based decision support system used for evaluating the probability of avalanche release underlines the statement of Casti (1992), that complexity is not an intrinsic property of the system but depends on what we want to “see”.

Avalanche dynamics: On the calculation of avalanche run-out many efforts are put in recently. The quality of statistical models, simple physical models and more advanced physical models will be compared in general and demonstrated on the event of the catastrophic avalanche of Galtuer. The results show that the consideration of stable and unstable parts of the system seems to be the key question to improve the quality of models. The integration of stochastic behaviour and uncertainty would be easier if this kind of system analysis would be done more seriously.

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Emissions and Fuel Economy Trade-Off for Hybrid Vehicles Using Fuzzy Logic

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Abstract

In this paper, a generalized fuzzy-logic controller is used to optimize the fuel economy and reduce the emissions of hybrid vehicles with parallel configuration. Using the driver input, the state of charge of the energy storage, the motor/generator speed, the current gear ratio and vehicle speed, a set of 44 rules have been developed, in a fuzzy controller, to effectively determine the power split between the electric machine and the internal combustion engine. The underlying theme of the fuzzy controller is to optimize the fuel flow and reduce NOx emission. The parameters in the fuzzy rules can be adjusted to trade-off the fuel economy and the NOx emission of the vehicle.
Simulation results are used to assess the performance of the controller. A forward-looking hybrid vehicle simulation model is used to implement the control strategies. By using fuzzy logic, trade-off between fuel economy and emission improvement has been shown.

Keywords: Hybrid vehicles; Energy management systems; Fuzzy control; Optimal power flow; Automotive control

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Physical Modelling

PLASTIC STRUCTURAL ANALYSIS UNDER STOCHASTIC UNCERTAINTY

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In plastic analysis of mechanical structures one has to maximize a load factor μ under a safety condition consisting of the equilibrium equation and the yield or strength condition.
A basic problem is that due to random material variations, random variations of the loadings, manufacturing and modelling errors, the material resistance or strength parameters of the structure, as e.g. the yield stresses, plastic capacities, etc., as well as the external loads and certain cost factors, are not given, fixed quantities, but random variables having a certain probability distribution.
In order to omit - as far as possible - a structural weakness and therefore a possible failure or severe damages and then very expensive repair or reconstruction actions, the available a priori information (e.g. certain moments) about the random variations of the unknown technical parameters and loadings should be taken into account from the beginning. Hence, in order to get **robust** limit load factors μ with respect to random parameter variations, the original limit analysis/shakedown analysis problem with random parameters must be replaced by an appropriate deterministic substitute problem.

Starting from the basic structural safety conditions, we have to consider the convex or linear yield/strength condition and the linear equilibrium equation involving the member forces and bending moments or the generic stress vectors in the chosen reference or "check" points of the structure. Based on the static (lower bound or safe) theorem and the kinematic (upper bound or unsafe) theorem, expected cost-based plastic analysis problems (CBO) minimizing, bounding, resp., the (total) expected costs including the expected costs of failure can be described in the framework of a two-stage stochastic (linear) program (SLP) "with complete fixed recourse", i.e., with a special staircase structure.
For finding this representation, the structural failure is evaluated first by a scalar function s^* which is the minimum value function of a convex or linear program based on the static/kinematic theorem of the structure. This limit state function of the limit load/shakedown analysis problem can be interpreted as the resistance reserve (positive or negative) of the structure based on the present layout. As an important basic property of s^*, the affine-linearity of s^* with respect to the load factor μ is shown. Then, the corresponding cost function c^* for the cost evaluation of inadmissible stress states can be represented also by the minimum value function of a certain convex or linear program. Appropriate cost factors in the cost/loss functions are obtained, e.g. for trusses or frames, by taking into account the elastic/plastic strains in the elements of the structure caused by the member forces or bending moments of the structure.
Due to this representation of s^* and c^*, for given material and load parameters, an explicit analytical representation of the limit load factor μ^* can be derived which enables then the computation of the sensitivities of μ^* with respect to the material and loading parameters.

For the computation of robust limit load factors, we consider the following basic dual deterministic substitute problems:

i) Maximize the load factor μ subject to expected failure/recourse cost constraints;

ii) Minimize the expected total costs (cost for missing carrying capacity plus failure/recourse costs).

For special (quadratic) loss functions, approximate robust limit load/shakedown factors are determined analytically. In case of piecewise linear, convex cost functions, robust limit load/shakedown factors can be determined numerically by solving a linear program having a dual decomposition date structure. The basic properties of this method are examined, and numerical examples are given.

RELATIVISTIC DYNAMICS AND THE ENTROPY MAXIMIZATION PRINCIPLE

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Abstract. In Statistical Physics the distribution of the momenta of the micro-constituents of a fluid at a thermal equilibrium is derived from the entropy maximization principle. The question whether the validity of this principle is a consequence of the prevailing dynamics of the micro-constituents is mathematically open.

In the present contribution this problem is reified for the context of the relativistic dynamics that are imposed on a complex virtual system of micro-constituents.

We introduce the notion of the Boltzmann-Gibbs entropy in a measure-theoretic set-up an reformulate a theorem from the literature which is crucial for the determination of the entropy maximizing distribution of the momenta of micro-constituents. The theorem is then applied to obtain a prediction of the behavior of a 2-dimensional relativistic gas consisting of hard disks.

An event oriented implementational concept for the dynamics of the gas is also presented; this concept was used for the design of a computer experiment which is now available through the internet as an interactive applet.

We report on the outcomes of computer experiments that were evaluated with tools from Nonparametric Statistics; the reader, however, is invited to gain her/his own experience with the offered applet.

VARIATIONAL MODELLING FOR INTEGRATED OPTICAL DEVICES

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In modern optical telecommunication all-optical devices are used to manipulate light for various purposes. These (nano- and micro-meter scale) devices exploit interference properties to manipulate the light that is transported to and from the device through waveguides; for instance, a filter will select a specific wavelength from a broad spectrum of light. Characteristic is that these problems have to be modelled on unbounded domains. Although the devices (and surrounding region where the changes in light are most essential) are small, the presence of waveguides and the unavoidable radiation in unknown directions makes it difficult to 'confine' the problem, while this is desirable for mathematical analysis and numerical calculations.
In this paper we describe a practical way to confine the problem (possibly approximative) by exploiting the variational structure of the problem. The methods are motivated and are well suited to obtain numerical discretizations, like Finite-Element-Methods, on bounded domains while taking care that radiation will not be reflected at the artificial numerical boundary.
Restricting to planar structures, and to materials that are lossless (non-dissipative), nonmagnetic and linear, Mawell's equations reduce for monochromatic light to inhomogeneous Helmholtz equations, which uncouple into a set of two scalar equations for two polarizations. Restricting to TE-polarization, the scalar equation for the spatially dependent part u of the perpendicular component of the electromagnetic field is the Helmholtz equation which is the Euler - Lagrange equation of the Helmholtz functional

$$\mathcal{L}(u) = \int_\Omega \frac{1}{2}\left[|\nabla u|^2 - k_0^2 n^2 |u|^2\right]$$

where $k_0 = \omega/c$ with c the speed of light in vacuum, and n is the index of refraction of the materials and characterizes the geometry of the device.
The variational formulation produces automatically the desired interface conditions at boundaries between different materials. The full description should be considered on the whole plane, and in- or outflux conditions should be specified. Such conditions will restrict, but not completely determine, the behaviour of the function at infinity. For two applications we investigate how the formulation can be adjusted to obtain formulations on bounded domains, for which appropriate boundary conditions will have to be supplemented. (Various extensions, such as to incorporate Kerr-nonlinear effects, can be considered.)
The first problem is a 1D reflection problem with specified influx from a uniform medium; this incoming wave will partially be reflected and partially be transmitted by index variations that are supposed to be restricted to a confined interval. Correct Transparant-Influx boundary conditions at the boundaries of the confined interval will arise from introducing a value-function to the confined functional (specifying the influx) and taking variations of the free boundaries.
For a 2D waveguide with a uniform exterior and arbitrary interior index properties, the guided modes will be found from a variational formulation of the eigenvalue problem with correct boundary conditions at the boundary of the waveguide itself.
Detailed numerical calculations for extensions of these applications have been reported elsewhere, see e.g. [1, 2].

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MATHEMATICAL ANALYSIS OF AN EVAPORATING CRYSTALLIZATION PROCESS

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In sugar production an optimal process control for the crystallization operation is of great importance regarding the balance of mass and energy flows. The objective is to minimize the steam consumption, to use the available capacities perfectly and at last to increase the quality of sugar. Thereby the duration of the crystallization process as well as an equable supersaturation during the crystallization process are the most important variables influencing the sugar quality parameters.

Crystallization is one of the basic operations of thermal process engineering and describes the procedure where crystals are formed from a previously homogeneous system. Crystallization can take place from the solid as well as from the liquid and gaseous phases. In sugar production the evaporating crystallization from solutions, especially from aqueous solutions, is very important. To enable a crystallization process in a sugar solution the saturation solubility has to be exceeded. This supersaturation is produced by the evaporation of water.

The control of crystallization processes needs a deep understanding of the crystallization process itself. To develop a batch control for the crystallization of sugar a non-linear 4th order model is derived using mass and energy balances. The presentation will demonstrate the important steps to draw up the balances for the main mass flows around the crystallizer, illustrated in the figure. Special emphasis will be given to the mathematical description of the mass transfer flow from liquid sugar to solid (crystal) sugar. There have been several research activities to quantify the mass transfer in crystallization processes. Though many scientists agree that the driving force of crystallization is the difference in concentration between saturated and supersaturated solution and that the transferred mass flow further depends on the size of phase interface between liquid and solid, as well as on a mass transfer coefficient, there is still no clear approach to calculate it. In this contribution the mass transfer flow is estimated with the theory of analogy by means of the relationship between the *Reynolds, Schmidt* and *Sherwood* normalized numbers.

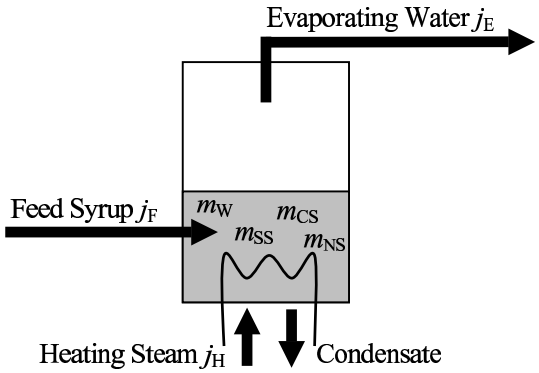

Figure: *Main mass flows in the crystallizer*

A second part of the presentation will deal with the model implementation in Matlab/Simulink. To proof the quality of the developed crystallization model it was validated against a real sugar production plant by several simulations. Comparison with measured values from the real process shows a very good conformity. It will be shown that the essential characteristics of the complex crystallization process can be reproduced in the nonlinear dynamic mathematical model. The validated model was used to improve the control strategy running during the crystal growth phase and controller parameters were optimized in simulations. Furthermore it will be presented that the attained perceptions of the model simulations can be successfully transferred to a real crystallization process in a big sugar production plant. Hence the mass and energy flows during the sugar crystallization process could be significantly balanced, without running risky experiments at the real production process. This contribution represents an important step to a sugar crystallization process, which is better understood, and much more balanced than before.

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A SIMPLE QUANTUM MECHANICAL MODEL FOR DERIVING THE ENERGY FUNCTION OF n-COMPONENT SYSTEMS

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We consider a general system consisting of n components, like ensembles of atoms or molecules together with forces centrally binding to components or due to interactions, whose quantities are known.
A state of our n-component system is defined as the superposition $\psi = x_1\psi_1 + \ldots + x_n\psi_n$ of the states $\psi_i, i = 1, 2, \ldots, n$, where ψ_i is the state the system will adopt if the only force which has some effect on the system is the force centrally binding to component i. We assume $\psi_i = \mathbf{e}_i$ (i-th unit vector of $\mathbb{R}^n$) and identify ψ with the vector $(x_1, \ldots, x_n) \in \mathbb{R}^n$. – Our definition includes the special case of physically interpretable states, for which we assume $\sum_{i=1}^n x_i^2 = 1$.
An observable on the system is defined as a continuous function of $\mathbb{R}^n$ to $\mathbb{R}$. Next we assume that for the energy observable F we only know the values

$$F(\mathbf{e}_i) = \alpha_i, \quad i = 1, 2, \ldots, n \quad \text{and} \tag{1}$$

$$F(\frac{1}{\sqrt{2}}(\mathbf{e}_i \pm \mathbf{e}_j)) = \frac{\alpha_i + \alpha_j}{2} \pm \beta_{ij} \tag{2}$$

for those pairs (i, j) with $i \neq j$, for which the components i and j interact.
The α_i (< 0) represent the forces centrally binding to components i and $\beta_{ij} = \beta_{ji}$ (< 0) are the values of the forces of interactions between i and j, added or subtracted depending whether these forces are in parallel or repel each other, respectively.
From equations (1) and (2) we infer

$$F(\mathbf{x} + \mathbf{y}) + F(\mathbf{x} - \mathbf{y}) = F(\sqrt{2}\mathbf{x}) + F(\sqrt{2}\mathbf{y}) \tag{3}$$

for all $\mathbf{x} = \frac{1}{\sqrt{2}}\mathbf{e}_i$, $\mathbf{y} = \frac{1}{\sqrt{2}}\mathbf{e}_j$ for which components i and j interact.

Theorem 1 *Let F be an observable satisfying the conditions (1) and (2) and assume $F(\mathbf{0}) = 0$. Then F can be uniquely extended to $\mathbb{R}^n$ such that equation (3) holds for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$.*

It is shown that the unique extension of F is a quadratic form $\sum_{i,j=1}^n b_{ij}x_ix_j$ with $b_{ii} = \alpha_i$, $b_{ij} = \beta_{ij}$, if the components i and j interact, and $b_{ij} = 0$ elsewhere.
The eigenvalues of the symmetric matrix (b_{ij}) then determine the energy levels of the system in agreement with the standard Hückel molecular theory (cf. eg. [2], [1]).

Further, *concepts of stability* are introduced. In particular, an n-component system is called Δ_c-stable if for all triples i, j, k with $b_{ij}, b_{jk}, b_{ik} \neq 0$ where the b_{ij} are defined as above the triangle inequality $|b_{ik}| \leq |b_{ij}| + |b_{jk}|$ holds.

Theorem 2 *Assume $b_{ii} < b_{ij}$ for $i \neq j$, $i, j \in \{1, 2, \ldots, n\}$. Then the n-component system is Δ_c-stable if and only if $2b_{ij} \leq b_{ii}$ for all $i, j \in \{1, 2, \ldots, n\}$ with $i \neq j$ and $b_{ij} \neq 0$.*

Theorem 2 can be used to determine the stability or non-stability of some molecules like cyclobutadien (non-stable) or benzen (stable). The obtained results are in agreement with known experimental data.

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VALIDATION OF THE SIMULATION MODEL FOR THE RADIATION VIEW-FACTOR CALCULATION

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In the paper the validation procedure of the simulation model for radiation view-factor calculation in industrial furnaces is presented. The simulation model bases upon the Monte Carlo method and allows determination of generalized view-factor matrix for general furnace geometry consisted of rectangle surfaces.

The Monte Carlo is a statistical simulation method, therefore the results in general contain fluctuations about a mean value. For some simple problems it is possible to calculate directly the probability that the obtained result lies by less than a certain amount from the correct answer. Even if it is possible to directly calculate the confidence level for more complicated situations, this would not take into account the pseudorandomness of the computer-generated random numbers [3]. For radiative heat transfer calculations the most straightforward way of estimating the error associated with the sampling result is to break up the result into number of subsamples. The subsamples may then be treated as if they were independent experimental measurements of the same quantity. The variance σ can then be calculated and the central limit theorem can be applied to determine the confidence that the correct answer lies within the limits around the mean value. In the model the $2\sigma_I$ interval is used to assure the 95.5% confidence.

For the validation of the simulation model and for the analysis of the uncertainty of calculated view-factor, two-surface geometry, which can be solved analytically was used. The uncertainty in Monte Carlo results depends also on the particular geometry under study [1]. The uncertainty increases as receiving surface gets smaller at unchanged emitting surface and number of photons. Therefore it is important to choose comparable worst-case condition of surface dimensions as they are in the furnace enclosure. The simulation has been performed using different numbers of emitted photons. The uncertainty 2σ is calculated for every number of emitted photons used in the simulation. It has been found out that for the particular furnace geometry 10^6photons/m^2 should be used to reach the uncertainty $\pm 1\%$.

The model has been tested using two different random number generators: the standard C generator "rand" and the "Mersenne Twister"[2] generator. The simulation has been performed using different numbers of emitted photons with both random number generators. The uncertainty 2σ is then calculated for every number of emitted photons used in the simulation. The results confirm that standard random number generators can be used in Monte-Carlo thermal-radiation simulation of reheating furnace.

The symmetry test of the simulation model has been performed using five-surface symmetric geometry. The simulation of view-factors from the base surface to other surfaces has been made using 10^6photons/m^2. The simulation results show that the symmetry of results is within the prescribed uncertainty.

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MODELLING THERMAL BUILDING DYNAMICS WITH MODELICA

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During the past decades, heating and air conditioning systems were usually designed and consequently oversized according to simplified, mostly static calculating procedures. The increase in primary energy costs and increased demand on comfort forced engineers to change the customary procedure. Thus the comprehensive dynamic simulation of building and system dynamics as well as user behaviour and external influences through the outdoor climate play an increasingly important role in planning and dimensioning buildings and their HVAC systems.

It is true, there is a great variety of simulation tools – mostly conceived for architects and building engineers. These tools pretend to offer a high transparency and flexibility through their menu-guided modelling but can often not be completely overlooked by the user as to their numeric methods, the effects considered and approximations applied. Operations going beyond what is provided by the menu are either not possible or can only be realized at great expense.

The new *Modelica* building model library opens up another way. Using an open simulation system providing the mathematical formalism, the model specification is done by the description of the basic physical laws which describe the relevant properties. An object-oriented, acausal language like *Modelica (http://www.modelica.org)* offers perfect conditions for this concept. A complex process model can be clearly arranged out of several hierarchically structured components (see figure). These components are coupled via cut variables – potentials and flow quantities – having a physical meaning (e.g. temperature, pressure, mass and heat flow).

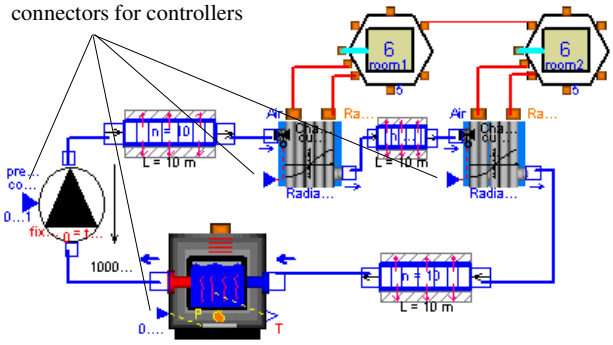

***Figure**: Two rooms with hot water heating system*

In the context of our work, a model library for the simulation of thermal building behaviour has been developed in *Modelica*. Due to the interdisciplinary character of building simulation, this domain is an ideal application of *Modelica*. Our modelling and simulation environment is *Dymola* (starting with version *4.1a*) by *Dynasim (http://www.dynasim.se)*.

The new model library is divided into four sublibraries:

- *Building* (describing heat storage and transmission within and between basic building structures),
- *Weather* (proving weather-related influences, especially those caused by solar radiation),
- *Heating* (modelling hot water heating systems),
- *Controller* (emulating the behaviour of conventional controllers and Fuzzy Controllers).

The building models have been validated in exemplary configurations against the building simulation system *TRNSYS* [1].

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CONCENTRATED HEAT SOURCES IN A HEAT CONDUCTING ROD

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The paper shall demonstrate how concentrated source terms can be included by Delta functions in models with distributed parameters and, moreover, that the abstraction of sharply concentrated quantities leads to decisive numeric advantages. The system of differential equations loses its stiffness here at the method of lines. The eigenvalues of the Jacobian matrix (A-matrix) show that it becomes stiffer with decreasing e since the heat capacity of the source is reduced spatially.
Physics knows abstractions without spatial or temporal extension, called sharply concentrated quantities here, like the point mass, a punctually attacking force or an immediate force impulse. In contrast to narrowly concentrated quantities of finite breadth the description is dropped in this section, what means an essential simplification.
For the presentation of narrowly concentrated quantities serves the Delta-epsilon function $d_e(x,t)$ which describes the sharply concentrated case after the limiting process $e \to 0$. In earlier projects the influence of sharply concentrated quantities in continuous models consisting of ordinary differential equations (ODE) had been investigated [1]. For the method used a characteristic feature is that an analytical integration of the differential equation with Delta function was put in front of the numeric treatment from which a system of two differential equations results [2]. The Delta function changes into a step function this way, which can be represented by a discrete event.

The presented contribution forms an expansion on models with distributed parameters. Concentrated source terms are described by Delta functions, and before the numeric treatment an integration is carried out over its area. We get, for example, a heat balance of the heat source from the partial differential equation, which we could win also from physical considerations.
Solution procedure is the method of lines. It changes the partial heat conduction equation into a system of ODEs with constant coefficients. The heat source of the breadth $2e$ is modeled by a Dirac Delta-epsilon function of space independent power density. The space integral above yields a differential equation of first order for its middle temperature. This is also a differential equation for the temperature in the source centre at adequately small e ($e << 1$). Space derivatives are approximated here and in the ODEs of the other grid points by finite differences. The negative, real eigenvalues can be different by several orders of magnitude. The numeric integration will require a Gear method here.
If we carry out the limiting process, then the stiffness of the system disappears since the temperature in the source follows from an algebraic relation now. For the numeric integration an explicit one-step method suffices in this case. The sharply concentrated borderline case can be an approximation for a class of narrowly concentrated terms, as a numeric comparison shows.

The regarded case of concentrated heat sources in the heat conducting rod is of exemplary character for partial differential equations with the time variable, one independent space variable, and spatially concentrated sources. The eigenvalue analysis also proves that the large differences of the eigen-frequencies at concentrated forces on the swinging string disappear in the borderline case [3]. Greater integration steps are permitted now.

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Modeling for Nonlinear Control of Rapid Thermal Anneal in RTP

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Abstract

The semiconductor device becomes highly integrated and has speeded up year by year. With that the technology to form ultra shallow pn junctions in MOS transistor becomes indispensable. The procedure for making pn junctions is composed of (i) “ion implantation” to dope impurity ion into a substrate, and (ii) “activation annealing” to activate the ion. At the stage of (ii), it is important to reduce the annealing time. This is because impurity ion, which is highly integrated and doped shallowly, is diffused in the depth direction of the substrate by heating for a long time, resulting in pn junctions formed more deeply.

RTP is the single wafer Rapid Thermal Processor with halogen lamps as the heating source, which enables to shorten the heating time with high temperature ramp-up and ramp-down rate. Among RTA(annealing process using RTP), the process whose ramp-up and down profile shows sharp fluctuation is called ”Spike RTA”. It has gained attention as one of the forefront technologies to form ultra shallow pn junctions. The current feedback PID control, however, has difficulty in following the reference temperature behind higher ramp-up rate of Spike RTA. As the ramp rate in Spike RTA rises higher, the current feedback PID control becomes difficult to track a given reference temperature trajectory. There are two reasons for the difficulty; (i) large response delay of halogen lamps which are the source of heating, and (ii) nonlinearity caused by the radiant heating. Generally speaking, the model using a feed forward controller is effective to compensate for these characters, but a highly accurate model is required to obtain high tracking performance. This study develops nonlinear models of the halogen lamp and the silicon wafer based on the physical equation of radiant thermal transport in a form which does not require the temperature data of the filament for parameter identification. Actually the halogen lamp model has only one parameter needed to identify.

In advance of identification of the only one parameter, we have to consider adjustment of the power balance to make the surface temperature of the wafer uniform. By minimizing the standard deviation of the distribution of the oxide film thickness, we are able to improve the uniformity of the distribution.

To identify the parameter of the model of the halogen lamp we apply a piecewise constant electric power and acquire response data of radiation energy from the lamp measured by a photodiode from which we can determine the only one parameter of the model of the halogen lamp. Experiments on the steady state relationship between wafer temperature and electric power of the lamp prove that power 4 of absolute temperature of the wafer and the electrical power of the lamp have a linear relation the intersection and gradient of which can determine the unknown parameter in the model of the wafer.

Identification accuracy of the nonlinear model developed in this paper is verified by comparing with the linear model in transient response experiments which prove very good tracking of the model developed.

Nonlinear feed forward controller is composed based on the developed nonlinear model. The control experimentations for RTA and Spike RTA processes are conducted with the latest rapid thermal processor applied this controller system. The result of this experimentation indicates that the tracking error is significantly improved compared to the usual feedback controller in each process. The repeatability of the top temperature is within $2°C$, which is sufficient for practical use. Furthermore, from the experiment, it is confirmed that developed model and controller have the performance which is robust for the characteristic difference of the wafer.

MODELLING OF THE PRODUCTION OF MICROWELLS

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In many fields of modern engineering miniaturization has become more and more important. The same holds for different fields in chemistry. Even though there are already some existing methods for the formation of surfaces, not all demands can be satisfied by one of these procedures in total. Hence new methods in this field are still of high interest for research and industrial production.

A new method for the production of microwells is presently under experimental and, by means of simulation, theoretical study. As an example for the new method, a small drop of toluene is placed on a plate of polystyrene. After the drying process the surface is well shaped as a mask for microlenses or to perform chemical reactions and processes such as crystallization or dissolving.

A mathematical model has been developed in order to understand the process of the microwell formation. The model recognises the following physical and chemical effects of the system:

1. growth of the drop on the substrate,
2. evaporation process of the solvent,
3. dissolving process of the substrate,
4. flow rate in the evaporating drop caused by the pinning effect, including its vertical profile,
5. increase of the concentration of dissolved material followed by precipitation.

An understanding of the influence of parameters such as concentration of the solvent in the surroundings, different solvents, mixtures of solvents, etc. is of high interest with respect to the optimization of the whole process. Thus it is also possible to think about forming micro landscapes on demand for chemical processes.

It could be shown, that the duration of drop growth and the flow rate of the solvent, respectively, have a strong influence on the depth and form of the profile of the microwells. Though the model for the simulation here was quite simple, the simulated results are in good agreement with experimental results.

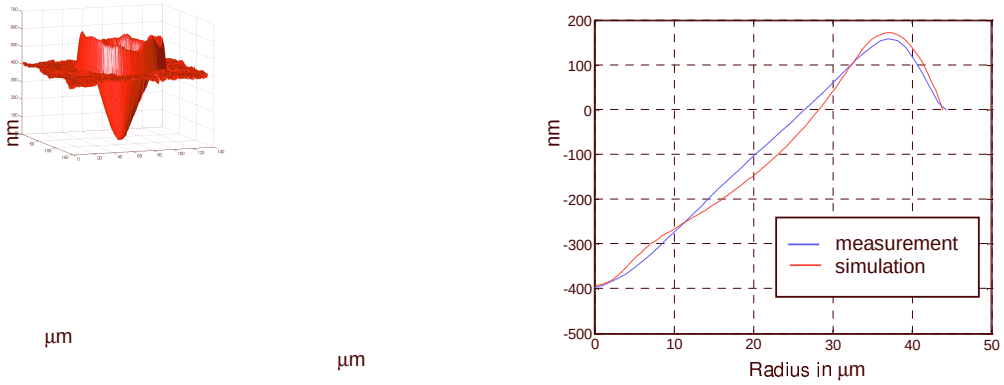

Fig. 1: AFM-image of a microwell (left) and comparison of measured and simulated data (note different scales).

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MODELING OF SEGREGATION ON MATERIAL INTERFACES BY MEANS OF THE FINITE ELEMENT METHOD

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A novel approach for segregation modeling on interfaces of three-dimensional structures is described. A numerical scheme is introduced as an extension to the standard finite element scheme for the diffusion problem. A simulation example for the case of an intrinsic dopant diffusion condition is presented.
We consider two segments S_0 and S_1 of different material connected with the plane interface I. The single species with the concentration C spreads out under intrinsic dopant diffusion condition in both segments S_0 and S_1 with constant but different diffusivities D_0 and D_1, respectively. In that case the diffusion governing equations in each of the segments can be written as

$$D_i \Delta C = \frac{\partial C}{\partial t}, \quad i = 0, 1. \tag{1}$$

At the interface I the species flux J_{ij} from segment S_i to segment S_j (normal to the interface) is given by [1,2,3]

$$J_{ij} = h\Big(C^i - \frac{C^j}{m}\Big), \tag{2}$$

where h is the transport coefficient, m the segregation coefficient, and C^i and C^j are the species concentrations in segments S_i and S_j. On the outside boundaries of the S_0 and S_1, the homogenous Neumann boundary condition for the dopant species C is assumed. Segregation, i.e. mass transport of species C through the interface I, is modeled by (2) and together with (1) completes the model considered in this work. The basic idea of our approach is to use the term $\int_{\Gamma_\Theta} \frac{\partial C}{\partial n} N_k \, d\Gamma$ which appears by setting of weak formulation of the problem to introduce the influence of the species flux from the neighboring segment area by applying the segregation flux formula (2)

$$\int\limits_{\Gamma_\Theta} \frac{\partial C}{\partial n} N_k \, d\Gamma = \int\limits_{\Gamma_\Theta} h\Big(C^1 - \frac{C^0}{m}\Big) N_k \, d\Gamma. \tag{3}$$

where Γ_Θ is the part of the interfacial area I between the segments and N_k linear form function. Basically the numerical procedure consist of two parts: First we assemble stiffness matrix of both segments as separated problems and secondly we add interfacial contributions which are derived from the discretization of (3).
For the one-dimensional case an analytical solution of the problem is derived. The results of the numerical procedure are evaluated with the analytical solution and with which it exhibits very good agreement. The $3D$ example of simulated species diffusion exhibits also accurate physical behavior on the material interface. The calculation of the species mass in both segments has shown that the presented numerical scheme complies with the mass conservation low very well.

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FEMLAB - a General Finite Element Package for Equation-Based Modeling

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1. Introduction

Computing hardware, computational algorithms, and user interfaces have seen major advances over the last 25 years. So much so that resources required for advanced scientific computing are now readily available to researchers, engineers, educators, and students. Harnessing these resources, however, remains a challenge. There are clear engineering needs for effective deployment of robust, flexible, and open schemes in usable and intuitive packages for research and teaching. The talk focuses on the development of FEMLAB, a partial-differential-equation-(PDE-) based modeling environment for multiphysics. Issues that will be addressed include graphical interfaces, numerical algorithms, symbolic equation specification, and multiphysics coupling.

2. Symbolical Treatment of General Sytems of PDEs

The first challenge in the design of a general PDE solver is to design an interface, graphical or code-based, that is able to handle symbolical expressions for arbitrary systems of PDEs. The purpose of this interface is to swiftly transfer the symbolical expressions to a form that can be used to generate the finite element code. In this paper, three different alternatives for definition of systems for PDEs are presented and these are briefly described below.

The first alternative is to enter a system of PDEs through a so-called coefficient form. This implies that the coefficients in front of different operators are defined in the graphical user interface or in the code-based interface. It is used for linear problems or 'almost' linear problems and uses an approximation of the Jacobian matrix.

The second option is the so-called general form. Here, the system of PDEs is written in a divergence. The general form is used for nonlinear problems, since it calculates the analytical expressions for the components in the Jacobian matrix.

The so-called weak form presents the last alternative for the definition of the, where it is possible to define equations using an integral formulation. The weak form is at the heart of the finite element method, and gives complete control of the finite element model. The three different 'forms' for translating analytical expressions to code have been proven to be very flexible and they are able to interpret almost any system of PDEs emerging in engineering and science.

3. Systems of PDEs in Terms of Physical Expressions

In most cases, engineers and scientist need some assistance in the definition of the PDEs and boundary conditions that describe a certain system or phenomenon. For this purpose, a 'library' of PDEs is included in FEMLAB, which sets up the most common systems of PDEs with the corresponding and most applicable set of boundary conditions. Each pre-defined description or phenomena is denoted application mode, e.g. the Navier-Stokes application mode defines the Navier-Stokes equations with the most common boundary conditions that can be individually selected for each boundary.

The program is also designed to combine different application modes in one single model. This implies that its is possible to define the coefficients, sources, sinks, or any other term in the pre-defined system of equations, as arbitrary functions of the dependent variables and their derivatives. This feature is denoted 'multiphysics' and gives virtually unlimited combinations.

4. Non-local Couplings

In engineering and science, a model often involves descriptions in different dimensions and in different coordinate systems. In order to handle these types of couplings, the original multiphysics feature was extended to handle coupled systems of PDEs including different sets of independent variables and geometries. This also implies that it is able to freely couple ODEs with PDEs through projections, reductions, integral expression, etc.

MATHEMATICAL MODEL FOR TORSIONAL SURFACE WAVES

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ABSTRACT

The study of surface waves is important to seismologists due to its application to know inside the earth and its possible use in study of earth quake, its prediction and effect.
The information on the propagation of two well known surface waves inside the earth during earthquake namely, Rayleigh and Love waves are available. In addition to the above mentioned waves the earthquake generates another type of surface wave in heterogeneous earth. These waves produce twist in the medium and hence may be called as Torsional wave. Due to its nature of propagation the damage due to earthquake may be more as compared to Rayleigh and Love waves. However, torsional waves have not been studied widely and due to its very nature of construction of seismogram (which plots only horozontal or vertical displacement) , these waves are not well recorded. Lord Rayleigh [1945] on the basis of mathematical model arrived at the result that homogeneous earth does not allow torsional surface waves to propagate. Recently Vardoulakis [1984] has shown that non-homogeneous earth can propagate torsional surface waves. This inspires the preparation of this paper and mathematical model to study the torsional surface waves have been developed for different types of variation in density and rigidity. The effect of gravity and presence of initial stresses have also been studied in the model. Although extensive study on this wave has been made, quite a few are being presented in the paper.

Model I : Discusses the propagation of torsional surface waves in a homogeneous substratum over a heterogeneous half space with linearly varying rigidity and density. The velocities of torsional surface waves have been calculated numerically and are presented in a number of graphs. It is also observed that for a homogeneous stratum over a homogeneous half space, the velocity of torsional surface waves coincides with that of Love waves. For a non-homogeneous half space it is observed that the velocity of torsional surface waves is always higher than that of Love waves propagated in a homogeneous layer over a homogeneous half space. It is concluded that such a half space allows two wave fronts for torsional waves while a homogeneous half space has only one.

Model - II: Discuss the effect of gravity and initial stress on torsional surface waves in dry sandy medium, it has been observed that the sandy medium without support of a gravity field can not allow the propagation of torsional surface waves, where as the presence of a gravity field always supports the propagation of torsional surface waves regardless of whether the medium is elastic or dry sandy.

MODELLING AND SIMULATION OF AWS: A wave energy extractor

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The paper addresses the steps towards an efficient time domain simulation of a wave energy device called AWS. The Archimedes Wave Swing (AWS) is an innovative near shore device built to extract wave energy from the sea, operating in intermediate water depth. The system consists of an air filled chamber fixed to the seabed, open at the top, called the silo, and closed off by a moving cylindrical lid called floater. The gap between the silo and the floater acts as an air lock preventing water from flooding the silo. The ocean waves have enough energy to make the floater of the AWS moving up and down assuring an oscillatory vertical motion used to produce electrical energy through a linear translator electric generator. To be able to assure this heave motion, the interior of the AWS system is pressurised with air to act as an air spring.

The absorption of wave energy means that energy has to be removed from the waves by cancelling or at least by attenuating them when passing the energy-conversion device. Such cancellation or attenuation of waves can be realised by the oscillating floater, provided it generates cancelling waves, which oppose the passing and/or reflecting waves. For that the floater should displace in an oscillatory manner and with correct phase to match the global diffraction wave characteristics. The larger efficiency is obtained if the floater is in resonance with the wave, that is, the principal frequency of the wave agrees with the natural frequency of the floater and the damping introduced by the electrical generator equals the hydrodynamic damping at this frequency. The mechanical power required to damp this resonance oscillation is partially converted into electrical power being the remaining power artificially dissipated in water dampers whenever the power exceeds the availability of the electrical equipment.

The AWS is a complex dynamical system operating under strongly fluctuating random conditions determined by the sea state. It has inherent nonlinearities in some of its components, including the power conversion system, which generate non-harmonic forces when it undergoes harmonic motion. Therefore, conventional linear frequency domain modelling is no longer valid to study this system. Instead, time domain models must be developed for the all subsystems, including structural, mechanical, fluid dynamics and electromechanical components. Thus, a time domain simulation model proves to be a very useful tool for both the design of such a device and to predict its behaviour. To build a time domain simulation the dynamical model of AWS needs to be built taking into account the main hydrodynamic and mechanical phenomena present in the system. Since all components of AWS interact with each other, the overall performance can only be evaluated by simulating the complete system. The intervening forces will be modeled taking into account the underline physical phenomena. The external water pressure force will act as excitation force, being related with the incident wave, the diffraction force and the radiation forces due to the AWS motion.

Besides the inherent complexity associated to the nonlinear dynamics of the system components, in the time domain, a convolution integral is conventionally used to model the hydrodynamic diffraction and radiation forces, being the last one characterized in the frequency domain by the added mass and damping. However, this integral is relatively expensive to evaluate and difficult to use with efficient integration routines. Here an efficient methodology mixing frequency- and time-domain is introduced to deal with this problem. The transfer functions were first obtained from a numerical finite element code, as vectors containing the frequency response of the desired transfer functions. The data obtained is then used to identify the corresponding analytic form of the transfer functions, which is integrated in the time-domain model.

The force due to the internal air pressure will take into account the heat generated by the electrical generator and the heat dissipated around the structure. The simulator includes the slow and fast dynamics of the AWS behavior associated with the tide and the wave, respectively. Also, the control actions for the slow and fast dynamics will be explained and included in the time domain model.

Random seas will be generated to simulate these irregular waves because the principle of superposition is no longer valid since AWS is a nonlinear system.

Simulation results of the overall simulator will be presented.

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Methods

MODELLING OPERATION OF INTERMEDIATE STORAGE IN BATCH/CONTINUOUS PROCESSING SYSTEMS UNDER STOCHASTIC CONDITIONS

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The intermediate storage has important role in improving operating efficiency and fitting to each other of subsystems of different operational characteristics of processing systems. Most of the works dealing with such problems have dealt with intermediate storages in batch and semi-continuous systems [1,2], but the study of modelling and reliable sizing of an intermediate storage connecting batch and continuous subsystems in processing systems under general stochastic operation conditions is also of primary importance.

The object of the paper is present a mathematical model developed for describing operation of intermediate storage aiming to buffer the operational differences between the batch and continuous subsystems of processing systems under conditions of uncertain inputs and constant continuous demand of the material to be processed. The batch units transfer possibly different amounts of material to be processed in moments of time the intervals between which are of independent exponential distribution so that the numbers of transfer events form Poisson processes with intensities independently on the other input units. The amount of material filled into the storage during a transfer of a batch processing unit also may vary randomly, and these amounts are described by independent random variables having the same general distribution function. Under such circumstances, two important problems may be formulated:

- Knowing the operational characteristics of the subsystems, determine the volume of the intermediate storage not allowing overfill it.
- Determine the initial amount of material with which starting the production process the amount of material in the storage will not decrease behind some given level.

Based on the stochastic differential equation model of operation of the storage, two, a direct and an inverse, risk processes, and the corresponding non-ruin probabilities are formulated which provide a basis for the rational design of such an intermediate storage. The ruin probability of the direct risk process, used to design the size of the storage, satisfies a delay Volterra type integral equation, while the ruin probability of the inverse risk process, used to design the initial amount of material in the storage required for normal operation of the system, satisfies an advanced Fredholm type integral equation.

Analytical solutions as well as solutions by stochastic simulation of the integral equations of the model are derived and compared in the cases of constant and exponentially distributed amounts of material transferred by the input batch units. The solutions obtained by simulation approximate well the exact solutions, thus this method can be used reliably for rational design of an intermediate storage in such processing systems.

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Removing Internal Delays from a Continuous-Time Markov Process

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Modern systems tend to be more and more complex, hence resulting in large and complex models. The notion of decomposing a system into smaller subsystems is well known and results in systems that are easier to model. This requires

a- Designing the specification of the system as a product of several components and
b- Proving that the product of these components conforms to the requirements of the system, the original specification.

Designing a system as a product of several components requires some internal interaction between the components themselves. When the product of these components is made, these internal interactions are hidden; they represent internal state transitions, visible at the system boundary only as additional delays. As a step for checking whether the product obtained conforms with the original specification, algorithms have been considered for removing internal transitions from the component product, while preserving isomorphism between the machine before and after removing the internal transitions. Such algorithms have been deescribed for the cases of finite state machines, I/O automata [2,3,4]… But for the case of continuous-time Markov processes (CTMC), it has been proven that we can not remove the internal transitions (also called empty moves) from a CTMC and still obtain an isomorphism [1].

J. Hillston [1] reduced the number of empty moves in a CTMC while preserving an equivalence named "weak isomorphism".

In this paper, we introduce an algorithm to remove empty moves from a CTMC while preserving some kind of equivalence. The equivalence relation is named "average delay equivalence" or ADE, where, informally, two CTMCs are equivalent if they have the same traces, same probability of occurrence of traces, and same delay time spent on average, for a given initial trace, before a particular next interaction occurs.

A few examples for removing empty moves from a CTMC while assuring average trace equivalence are also provided in the paper.

In a companion paper in progress, we have proven that, if two CTMCs M and N are ADE, then they exhibit "similar" behavior at equilibrium. We have also shown that this property is very useful in modeling Markovian subsystems from a given Markovian specification.

In the first section of this paper we present some basic definitions needed in the course of the paper, then in the next section we present the algorithm to remove the empty moves from a CTMC as well the definition of the average delay equivalence. And finally, in the last section, we give two examples of continuous-time Markov models with empty moves and show how to apply the algorithm to remove the empty moves. We also give some suggestions for future work.

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DETERMINATION OF EMBEDDING DIMENSION USING MULTIPLE TIME SERIES BASED ON SINGULAR VALUE DECOMPOSITION

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In this paper, the extension of the approach of finding the embedding dimension of chaotic systems based on Singular Value Decomposition (SVD) by using *multiple* outputs is accomplished. A comparison study illustrates the superiority over single time series analysis.

In some practical applications, the only available data from the process is in the form of scalar or vector sequences of measurements. The reconstruction of a state space from a time series, which is equivalent to the original state space, is the first step in the nonlinear methods of time series analysis and modelling. This reconstruction can be done by embedding the time series data in a state space. To achieve this, there are some embedding theorems, one of the most popular of which is the Takens' theorem [2]. This theorem leads to the *method of delays,* reconstructing the space from delayed values of a univariate time series of that system. Generically a scalar time series is sufficient to compute the embedding dimension. But in practice, a single output time series sometimes does not have the proper reconstructability properties. Hence, in such cases using a univariate time series of system does not guarantee that the correct dimension for embedding space can be found. This deficiency can be overcome using multiple (output) time series of the process.

In this paper, the main goal is to show the superiority of using multiple channels of output data for computing the embedding dimension with respect to the scalar case. Among the methods for computing embedding dimension, here, the SVD approach [1] that previously introduced for extracting qualitative information from observed time series is considered. The main core of this approach is to obtain a basis for the embedding space such that the attractor can be modeled with invariant geometry in a subspace with fix dimension. It is essentially a linear method, but, the part which enable us to use it as a nonlinear approach is the determination and arranging the singular values and related eigenvectors of trajectory matrix. Since singular values are data dependent, the selection of sampling time and number of samples in each row of trajectory matrix is the first important issue.

Using simulation results of well-known chaotic processes, it is shown that the individual univariate output time series do not contain the necessary information to obtain the correct embedding dimension. This is called in this paper the *unreconstructibility* of the state space from univariate time series. For example, in the Rössler equations the Z variable has a structure that the fluctuations of behavior of the system can not be seen in a finite number of its samples and as it is shown in the simulations that the appropriate embedding dimension is not derived from it. To resolve this drawback, the above mentioned approach is extended to the multivariate case and simulation results are provided to present the results obtained for to the multivariate extension. Following as in the univariate case, a real symmetric covariance matrix is defined and it is easily shown that for a given multivariate time series, the embedded dimension can be selected as the rank of the defined covariance matrix. Although in the multivariate time series studies, the procedure is similar to the univariate case, however the cross-covariance of different time series appears in some elements of covariance matrix instead of the autocovariance functions of the single time series. These elements cause the increase in the order of the singular values because of their data dependence. Finally, the simulations of the Rössler equations are repeated by using multiple output data. For the Rössler system, the normalized singular values are calculated by using the time series of variables X and Z jointly in the extended SVD method, and it is shown that the embedding dimension is clearly n=3 which is exactly the dimension of the chaotic dynamical system.

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LOW ORDER TIME DELAY APPROXIMATION OF CONVENTIONAL LINEAR MODEL

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The objective of the paper is to point out remarkable potentials of low-order time-delay models in describing the plants, the dynamics of which are used to be classified as "higher order". Two original modifications of model identification approaches are presented: a procedure of successive integrations of the step response of the plant and the relay feedback test applied to a time delay model. The obtained low-order models allow direct application in control system design including the implementation on programmable controllers as a simple linkage of integrators and delayors. The basic form of the considered first-order model is as follows

$$T\frac{\mathrm{d}y(t)}{\mathrm{d}t} + y(t-\vartheta) = K\,u(t-\tau) \tag{1}$$

containing delay in both the input and the feedback, unlike the papers practically aimed at controller design for time-delay plants assuming a plant model with a delay in control input only. By means of the triple integration of the plant step response the following conditions for the model parameters T, ϑ, τ are obtained

$$(T-\vartheta+\tau)\,y_0(\infty) = y_I(\infty), \qquad (\vartheta^2-\tau^2)\frac{y_0(\infty)}{2} - (T-\vartheta)\,y_I(\infty) = -y_{II}(\infty) \tag{2}$$

$$(\tau^3-\vartheta^3)\frac{y_0(\infty)}{6} - \vartheta^2\frac{y_I(\infty)}{2} + (T-\vartheta)\,y_{II}(\infty) = y_{III}(\infty) \tag{3}$$

allowing an easy identification by means of solving this set. The identification procedure proves the ability of this model to fit a „higher order" dynamics (including the oscillatory systems with a sufficient damping) by means of a first order model only. Equation (1) can be considered as state equation of the model for the state variable y while its state in the instant t is given by the following segments: $\hat{y}\langle t-\vartheta, t\rangle, \hat{u}\langle t-\tau, t\rangle$. It is to realize that the conventional third-order model is also able to fit just three integral conditions. In this sense model (1) may be considered equivalent to a model given by an ordinary third order linear differential equation.
The second method of identifying the time-delay model with is based on adding a relay feedback that results in limit cycle oscillations. The frequency ω_u of these oscillations and the appropriate ultimate process gain k_u resulted in the following conditions for the first-order model parameters

$$\vartheta = \frac{\pi - \arccos\left(K\,k_u\cos(\omega_u\tau)\right)}{\omega_u}, \qquad T = \frac{\sin(\omega_u\vartheta) - \tan(\omega_u\tau)\cos(\omega_u\vartheta)}{\omega_u} \tag{4}$$

where the values k_u , ω_u , τ , K are estimated in another way. Unlike the higher order models the parameters of the suggested model a straight-forward connection with the transient properties of the plant to be described and due to this their preliminary values can be estimated from the plant response. The presented low-order time-delay models are favourable for further use in control system design, e.g. for extending the control schemes as internal model control (IMC), state feedback scheme, pole placement design etc. towards the time delay systems. Moreover, the models do not bring about problems with their PLC implementation.

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NUMERICAL METHOD-INDEPENDENT STRUCTURAL SOLVABILITY ANALYSIS OF DAE MODELS

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Dynamic lumped process models described by differential and algebraic equations (DAEs) are investigated in this paper. The structural analysis of these models form an important step in the model building procedure used for the determination of solvability properties of the model. This analysis includes the determination of such properties as the degrees of freedom, structural solvability, differential index, dynamic degrees of freedom and results in the decomposition of the model and the determination of the calculation path. As the result of the analysis the appropriate numerical method for solving the model can be chosen efficiently. Moreover, advices on how to improve the computational properties of the model by modifying its form or its specification can also be given.

Effective graph-theoretical methods have been proposed [1, 2] based on the analysis tools developed by Murota, et al. [3], for the determination of the most important solvability property of lumped dynamic models: the differential index. The properties of the dynamic representation graph of process models described by semi-explicit DAE-systems have also been analysed there in case of index 1 and higher index models. Besides of the algorithm of determining the differential index using the representation graph, a model modification method has also been proposed which results in a structurally solvable model in case of higher index models.

For the construction of dynamic representation graphs the most simple, single-step, explicit numerical method (the explicit Euler-method) has been assumed as the numerical solution procedure for the differential equations. However, implicit solution methods are used more frequently and efficiently for numerical solution of DAE-systems. Therefore our aim is to investigate the effect of the numerical solution procedure on the structure of dynamic representation graph of the DAE models by considering single-step implicit solution method. Moreover, an extended method for the construction of the so-called reduced graph is also aimed at.

It is shown that the representation graph with implicit solution methods has similar properties both in the case of index 1 and higher index models than with explicit numerical solution procedure. Therefore, the determination of differential index and the suggested model modification for higher index models can be done in a similar way.

It can be proven that the properties of the representation graph including the differential index of the models are independent of the assumption that a single-step, explicit or implicit numerical method is used for the solution of the differential equations.

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BOND GRAPHS IN MODEL MATCHING CONTROL

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Bond graphs have proven to provide a convenient framework for the network modelling of lumped parameter physical systems. This graphical modelling methodology is now firmly established in the literature (e.g. [4]). On the other hand, it safe to say that bond graph based *control* is not documented in detail. Some initial results can be found in [2]. Possible advantages of bond graphs in control are the following. The role of modelling is emphasised, so that physical reasoning may provide additional insight into the control problem. Secondly, relatively systematic procedures are obtained, which are directly ascribable to the structured modelling rules imposed by the bond graph. Lastly, the object–oriented nature of bond graphs readily allows complex systems to be modelled. This paper proposes a bond graph interpretation of the nonlinear Model Matching Problem (MMP), which is elaborated in [3]. More precisely, we deploy bond graph techniques to derive controllers that render the input–output behaviour of a plant identical to that of a specified model. In addition, the model will chosen to be structurally "close" to the plant, so that the MMP can be cast into the virtual actuation framework as reported in [2]. We recall the fact that bond graphs belong to the class of implicit port–Hamiltonian systems, which have proven to be invaluable for a deeper understanding of the geometric structure of certain energy conserving physical systems [1]. The application of bicausality allows us to find a decoupling controller with disturbance measurement, where by definition of the MMP, model inputs are considered to be disturbances. When the resulting controller is applied, we obtain port–Hamiltonian error dynamics, so that we can represent it with a bond graph. It is then possible to use bond graph arguments to stabilise the error dynamics. Furthermore, we use recent results of [5] on interconnection and damping assignment passivity–based control to provide additional energy shaping that is not immediately apparent from the bond graph. We do not develop a strict bond graph procedure, since we wish to retain flexibility, but we give a detailed example and show the various steps.

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POLYNOMIAL MATRIX FRACTIONS AS MODELS OF LINEAR SYSTEMS: THEORY AND SOFTWARE TOOLS

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In spite of the fact that transfer functions as ratios of two polynomials are generally considered a useful and natural description of linear time invariant systems in the single-input-single-output constellation (SISO), many authors ignore their multivariable (MIMO) counterpart – the polynomial matrix fractions (PMF). Instead, they often rely on the state-space theory completely in that case.

The reasons for this approach are mainly historical. Until recently, no reliable software for polynomial matrices was available and even the numerical difficulties related to these objects were not completely understood. Nevertheless, during several past years a great effort has been paid to this problematic. As a result, new stable routines for polynomials and polynomial matrix fractions related to modeling and control systems were developed, see [2][3][4] for instance, and a dedicated software tool, Polynomial Toolbox for MATLAB, has been released [1].

We show in our paper that it is often convenient to utilize polynomial matrix fractions for modeling linear MIMO systems since the PMF's are intimately related to linear differential equations. These equations can be, in turn, derived from the first (physical) principles. In view of this, the construction of a state-space representation presents an additional artificial step that is not necessary in many situations.

The paper is organized in the following manner. The theory of polynomial matrix fractions is introduced first. Both discrete-time and continuous-time linear MIMO systems are covered. Conversions between left and right PMF's are recalled and the relation of PMF's to higher order differential and difference equations is enlightened. Foolowing this introductory section, we present construction of a PMF model to a real-life physical system by means of an example. Based on this model, a MIMO controller is designed using the Polynomial Toolbox for MATLAB [1] to illustrate the usefulness of the obtained description in the control systems context. Finally, for simulation of the model and of the overall control loop, the PMF Block of the Polynomial Toolbox Library for SIMULINK [1] is addressed.

Keywords: Polynomial matrix fractions, algebraic design methods, software tools.

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039) A TAUBERIAN CLASS FOR REPRESENTATIONS OF FOURIER AND FOURIER-STIELTJES COEFFICIENTS

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Fourier series and its generalizations are an essential part of the background of scientists, engineers and more generally of mathematical modeling. Therefore the structure of Fourier coefficients as well as the various forms of convergence of the Fourier series are of great importance. In this paper we will define and use a Tauberian class to obtain a representation of Fourier and Fourier-Stieltjes coefficients.

Let $f \in L^1(\mathbf{T})$, where $\mathbf{T} = \dfrac{\mathbb{R}}{2\pi\mathbb{Z}}$ with $\mathbb{R}$ and $\mathbb{Z}$ the sets of real and integer numbers respectively. If $\{c(n)\}$ is a sequence of complex numbers, we define the general trigonometric series as

$$\sum_{|n|<\infty} c(n)e^{\text{int}} \quad \text{where} \quad i=\sqrt{-1}\,. \tag{1}$$

A non-decreasing sequence $\{R(n)\}$ of positive numbers is *-regularly varying if

$$\lim_{\lambda\to 1_{+0}} \overline{\lim_{n}} \frac{R([\lambda n])}{R(n)} \le 1 \quad \text{for} \quad \lambda > 1\,. \tag{2}$$

We will be working with the subclass of all *-regularly varying sequences defined by

$$R(n) = \exp\left(\alpha_n + \sum_{k=1}^{n} \frac{\beta_k}{k}\right) \tag{3}$$

and using the Tauberian class

$$\lim_{\lambda\to 1_{+0}} \overline{\lim_{n}} \left(H_{[\lambda n]}(c) - H_n(c)\right) = 0 \tag{4}$$

where

$$H_n(c) = \sum_{0\ne|k|\le n} |\Delta c(k)| \log|k| \tag{5}$$

is the convergence modulo, we will show that condition (4) is equivalent to the existence of an $h \in L^q(\mathbf{T})$, $q \ge 2$ such, that

$$c(k) = \begin{cases} \dfrac{1-\text{sgn}(k)}{2}c(-1) + \dfrac{1+\text{sgn}(k)}{2}c(0) \; - \displaystyle\sum_{j=\frac{1-\text{sgn}(k)}{2}}^{|k|-1} \hat{h}(j\,\text{sgn}(k))\,, \quad k \in \mathbb{Z} \\ \displaystyle\sum_{j=|k|}^{\infty} \hat{h}(j\,\text{sgn}(k))\,, \quad k \in \mathbb{Z} \quad \text{if } c(n) = o(1)\,,\ |n| \to \infty \end{cases} \tag{6}$$

with

$$\left|\hat{h}(n)\right| = \begin{cases} \dfrac{1}{\log|n|}\left(\log\dfrac{R_1(n)}{R_1(n-1)}\right) & \text{if} \quad n > n_0 \\ \dfrac{1}{\log|n|}\left(\log\dfrac{R_2(-n)}{R_2(-(n-1))}\right) & \text{if} \quad n < -n_0 \end{cases} \tag{7}$$

for some *-regularly varying sequences $\{R_1(n)\}$ and $\{R_2(n)\}$ of the form of (3) and some positive integer n_0.

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L_2-OPTIMAL BILINEARIZATION OF NONLINEAR SYSTEMS

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The approximation of nonlinear systems to be controlled by simpler mathematical models is common practice in control system design. In a first approach to control system design for nonlinear systems one uses a Jacobi linearization of the plant about an operating point in order to apply linear control theory for designing a linear controller. However, in many applications the resulting performance of the closed loop system is not satisfactory, since the linear approximation model does not take the nonlinear character of the plant into account. A solution to this problem is the application of nonlinear control design strategies such as feedback linearization (see [2]) yielding a nonlinear controller, which achieves desired properties for the closed loop system not only in a vicinity of the operating point. The design of this controller using nonlinear control theory may be rather involved and in most cases can only be carried out using computer algebra packages. In order to facilitate the design of nonlinear controllers it is reasonable to use a somewhat simpler nonlinear approximation model of the nonlinear plant, which reproduces the behaviour of the nonlinear system to be controlled in a suitable region about the operating point. An interesting class of systems for approximating nth order nonlinear affine input systems are bilinear systems of order higher than n. The simple structure of bilinear system allows of nonlinear controller design only involving the manipulation of constant matrices. A well known and systematic approach for obtaining bilinear systems of higher order is the *Carleman linearization* (see e.g. [3]). By introducing the monomials of the plant states as states of the bilinear system, one can successively improve the approximation at the expense of higher dimensionality of the resulting bilinear system. The main drawbacks of the Carleman linearization approach are, that it relies on a Taylor series expansion of the plant nonlinearities and that the state equations are derived by simply omitting monomials of higher order. As a consequence this leads to bilinear systems, that approximate the plant only locally even for a high approximation order. Furthermore no prediction of the region is possible, where the resulting bilinear system is an accurate approximation for the plant under consideration. Based on preliminary results in [1] this contribution presents the *L_2-optimal bilinearization* as a new systematic approach for obtaining bilinear approximation models for nonlinear systems, which uses the basic ideas of the Carleman linearization but circumvents its drawbacks. Different from the Carleman linearization the proposed bilinearization approximates the system nonlinearities by multivariable orthogonal polynomials with minimal L_2-error norm on a given multivariable interval in the state space. In order to get a bilinear system description the orthogonal polynomials are introduced as new system states. The operations needed for obtaining the corresponding state equations are all carried out with minimal L_2-error norm, such that the resulting bilinear system is a valid approximation of the nonlinear plant in a prespecified multivariable interval of the state space. Hence different from the Carleman linearization approach, one can specify the region, in which the bilinear model approximates the given nonlinear plant. Along with the derivation of the L_2-bilinearization approach a systematic design procedure for the application of this bilinearization method is provided. A nonlinear model of the Van de Vusse reactor is used to demonstrate the new bilinearization approach.

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038) A LINEARIZED SCHEME FOR THE NUMERICAL SOLUTION OF THE BOUSSINESQ EQUATION

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Two different linearized schemes are going to be examined to known from the bibliography methods (see Bratsos [1]-[2]) concerning the numerical solution of the Boussinesq (BS) nonlinear equation.
BS equation, which belongs to the KdV family of equations and describes shallow water waves propagating in both directions, is given by

$$u_{tt} = u_{xx} + \left(u^2\right)_{xx}^2 + q u_{xxxx} \; ; \quad L_0 < x < L_1, \; t > 0. \tag{1}$$

where $u = u(x,t)$ is an appropriate differentiable function and $|q| = 1$ is a real parameter, which, for $q = -1$ gives the *Good Boussinesq* or *well-posed* equation (GB), while for $q = 1$ the *Bad Boussinesq* or *ill-posed* equation (BB).

For the numerical solution of Eq. (1) the region $R = [L_0 < x < L_1] \times [t > 0]$ with its boundary ∂R consisting of the lines $x = L_0$, $x = L_1$ and $t = 0$ is covered with a rectangular mesh, G, of points with coordinates $(x,t) = (x_m, t_n) = (L_0 + mh,\, n\ell)$ for $m = 0, 1, ..., N+1$ and $n = 0, 1, ...$ Let $\mathbf{U}^n$ be the solution vector at (x_m, t_n) for $m = 1, 2, ..., N$. Then using finite-difference approximants for the time and the space derivatives and applying Eq. (1) to each interior point of G, it leads to a nonlinear system for the unknown solution vector $\mathbf{U}^{n+1}$.
To avoid solving the nonlinear system the following two types of linearization to the nonlinear term of the BS equation were used. In the first it was considered the approximation

$$\left(U_m^{n+1}\right)^2 \approx U_m^{n+1} U_0 \tag{2}$$

where U_0 an appropriate constant, while in the second the approximation

$$\left(U_m^{n+1}\right)^2 \approx 3\left(U_m^n\right)^2 - 2U_m^n U_m^{n-1} \tag{3}$$

based on Taylor's expansion of $\left(U_m^{n+1}\right)^2$ about the n-th time level was used.

BS equation was solved numerically for both linearizations defined by Eqs. (2)-(3) for the single-soliton wave to the problems proposed by Bratsos [1]-[2]. From the experiments it was deduced that the results obtained were more accurate than the published ones.

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Simplification of the Generalized State Equations

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The paper studies the problem of lowering the orders of input derivatives in nonlinear generalized state equations via generalized coordinate transformation. An alternative, more transparent and shorter proof is presented for the theorem, originally proved by Delaleau and Respondek [1], giving the necessary and sufficient conditions for existence of such transformation, in terms of commutativity of certain vector fields. The dual conditions in terms of 1-forms are given on the basis of the new proof.

The problem for finding the state coordinate transformation is discussed in detail. The new state variables can be defined as the solutions of a system of partial differential equations – the invariants of certain vector fields, satisfying the condition of Delaleau and Respondek [1]. Alternatively, the new state variables can be found by integrating of the integrable set of 1-forms as the maximal annihilator of mentioned vector fields. Is derived an algorithm to find these 1-forms, not necessary exact, and a system of first order partial differential equations for finding the integrating factors. The contribution is illustrated with an example of a crane, originally given in [1], but solved in alternative way.

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MODELLING SYSTEMS WITH SYMMETRY

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Symmetry is fundamental property of any phenomenon or process. This is also actual for a model, which describes a phenomenon or process. Moreover a model as mathematical abstraction is more idealized than its original, and may have higher order symmetry or several types of symmetry.
In this paper the method for analyzing and decomposing systems having symmetries under discrete groups of transformations is considered. The method is based on the theory of group representation. If dynamical system's structure is invariant under discrete group the system has decomposition, which can be realized without solving eigenvalue problem. For systems with visual cyclic symmetry decomposition helps to find special features of behaviour. A model of a system is considered of the form

$$\mathbf{y}(t) = \mathbf{A}(d/dt, \mathbf{a})\,\mathbf{x}(t),$$

where $\mathbf{x}(t) \in \mathbf{R}^n$ – input vector, $\mathbf{y}(t) \in \mathbf{R}^m$ - output vector, $\mathbf{R}^n$, $\mathbf{R}^m$ – corresponding linear vector spaces, $\mathbf{A}(d/dt, \mathbf{a})$ - differential operator having vector of parameters $\mathbf{a} \in \mathbf{R}^p$. Corresponding initial conditions are assumed for concrete form of operator **A**. Model (1) has symmetry under group G = {g} if the following condition of commuting is true:

$$\mathbf{T}(g)\mathbf{A}(d/dt, \mathbf{a}) = \mathbf{A}(d/dt, \mathbf{a})\,\mathbf{S}(g)$$

where S(g), T(g) are matrices of symmetry group representation in the spaces $\mathbf{R}^n$, $\mathbf{R}^m$ respectively. These matrices can be found as permutation matrices for finite groups.
Proposition. If a model has symmetry and its operator commutes with matrices of reducible symmetry group representation, the model can be decomposed to the set of independent sub-models of reduced dimensions.
Model decomposition is based on the decision of the problem of reducing group representation [4,5].
There exist coordinate transformations

$$\tilde{\mathbf{x}} = \mathbf{M}\mathbf{x}, \quad \tilde{\mathbf{y}} = \mathbf{N}\mathbf{y},$$

which transform initial model to equivalent model in canonical basis so that the model has block-diagonal structure

$$\tilde{\mathbf{A}} = diag\{\mathrm{A}_i \otimes \mathbf{E}_{l_i}, i = 1, 2, ..., q\},$$

q – number of non-equivalent irreducible representations of group **G**, having square matrices of l_j dimensions.
Special technique of constructing matrices **M** and **N** is proposed.
The paper contains an example demonstrating as applying symmetry on the stage of creating model as decomposition for the model. Various symmetrical motors layouts shown on the Figure 1are modeled.

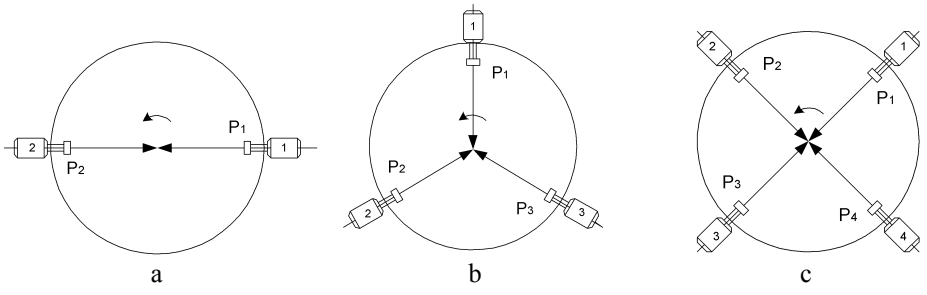

Figure 1. Various symmetrical motors layouts.

Symmetry properties of layouts depend on the verity of special assumptions about motors interactions. For cyclic symmetries of models of layouts having symmetry groups of $\mathbf{C}_n$, n = 2, 3, 4, corresponding decompositions are created and analysed.

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Large-scale linear model for optimal industrial investments: robust presolving analysis

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Which equipment should be bought for a given sum, to increase the profit of an industrial enterprise with a known specification of production within given limits of expenditure? This problem can be described as a large-scale linear program (LP) of a specific structure, as follows:

$$\begin{aligned} Ax - u &\leq l \\ 0 \leq x &\leq x_u \\ \sum c^T u &\leq d \\ f^T x &\rightarrow \max \end{aligned}$$

Here x is a vector of planned production with given upper bound x_u, f is a vector of profit per unit of the production, l is a vector of available resources, c is a vector of the prices of the resources, d is a given value of the available investments. All the coefficients in the input information have a box-constrained uncertainty.
An effective presolving system is needed to reduce its size by eliminating the redundent rows and columns. Presolving analysis with box-constrained uncertainty in the input information is presented in Ioslovich (2001). However, some specific problems can be considered in a more efficient way, taking into account their structure. In the present paper a robust presolving algorithm is considered for the mentioned problem. An algorhitm of robust evaluation of uncertain duals presented in Ioslovich and Gutman (2000) is used.

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Scalability Analysis and Synthesis of AQM Mechanisms

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I. Abstract

As the Internet evolves, the necessity of incorporating and exploiting some *active queue management* (AQM) mechanism is eliciting exciting research efforts (see, e.g., [2], [4], [5], [6] and references therein) over the past few years. A vital breakthrough was provided by [4] which gave a clean control theoretic interpretation of the RED, a widely used AQM protocol. It showed that RED control effectively amounts to using a *proportional*, i.e. P, controller with an additional low pass filter. Such a controller exhibits low closed loop bandwidth and, hence, a sluggish response [4]. Removal of the low pass filter from the RED design yields the classical P controller which has a higher closed loop bandwidth at the cost of reduced robustness [4]. A fuller analysis of TCP/RED protocol is given by [6] which effectively shows that the stability margin of a TCP/RED governed system reduces as the product of the closed loop delay and the network capacity increases; the same point is made in [5]. Now, a standard improvement over a P controller is a *proportional-integral*, i.e. PI, controller [1] and indeed [4] recently improved on the RED mechanism via a PI controller. It derives analytical results for a restrictive bottleneck network topology which runs an approximation of the TCP protocol. The PI controller in [4] suffers from a lack of antiwindup mechanism (see [1] and [3] for primers on classical controllers) and, furthermore, its robustness to link capacity and delay variations has not been characterized. Still, it paves way very admirably to analyze and synthesize robust AQM mechanisms, which is the objective of this paper. In this paper, we identify some of the critical factors which feature in the robustness analysis and adopt a standard control theoretic approach for the robustness analysis of a class of AQM mechanisms. Furthermore, we present a framework to synthesize a robust AQM mechanism given the perturbation bounds for theses factors. Briefly speaking, we solve the following two problems — 1. Given the round-trip time and the controller structure, find controller parameters which guarantee stability of the system, and 2. Find a range of round-trip time that guarantees stability of the system when controller parameters are given.

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Education

A CASE-STUDY BASED APPROACH TO MODELLING AND SIMULATION EDUCATION

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Along with five partner universities within the EU and USA, the University of Glasgow is a member of a consortium of universities involved in the USE-ME project (US-Europe Multicultural Education Alliance in Computer Science and Engineering). This project forms part of a larger international programme funded jointly by the European Commission Directorate General for Education and Culture and the US Government Education Directorate (FIPSE).

The aim of the USE-ME project is the development of international educational experiences for students undertaking graduate-level degree programmes involving computer modelling and simulation [3]. Some students are able to participate in exchanges that form one element of the project but there are many more who cannot take advantage of such periods of study abroad. Developments in e-learning are seen as providing a way of broadening the impact of the project through making teaching material developed in each partner institution available internationally to students studying elsewhere.

One of the goals involves development of new student-centred teaching material that, in the longer term, can form elements of a sustainable and shared e-learning environment. Developments at the University of Glasgow have been focussed mainly upon creating a number of multi-purpose case study presentations that are flexible in form and can be used as independent teaching units or can be combined readily with practical assignments and experimental work. How these case studies are applied depends on the educational aims and objectives of the programme within which they are being used.

The main emphasis in the case studies developed in Glasgow is on the modelling of nonlinear dynamic systems for engineering applications, model validation methodology, engineering applications of soft computing techniques and modelling applications involving automatic control. The case studies now available have all been developed for use initially within relevant modules at Master's degree level at the University of Glasgow but may be incorporated, without too much additional work, in an e-learning environment. Use of equipment for experimental work is a normal part of these case studies when carried out in Glasgow, but those working remotely can have access to files of experimental data. Such data can be used for model validation studies and other related investigations based on simulation.

The case studies outlined in the paper all relate to the development, validation and application of a nonlinear dynamic model of a coupled-tanks system. This equipment is of a type that is widely used for control engineering education. These particular case studies involve an enhancement of teaching material previously developed at the University of Glasgow[1,2]. There is a particularly strong emphasis on issues of model accuracy, model validation and model documentation in this group of case studies. It has been found that the open-ended nature of some of these investigations can encourage useful collaboration between students and it is hoped that ways can also be found within the e-learning environment of encouraging co-operation between students at different sites. This means that there is potential for international experience for students who are unable to spend periods of time outside their own university.

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A concept for a model server to integrate simulation models into web-based learning environments

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Important didactical elements for the composition of content within an authoring and learning environment are simulation models. They make the lessons vivid and efficient. For many application areas exist a large amount of simulation models which contain state-of-the-art knowledge and which are accepted by the according scientific community. This knowledge should be opened for the authors and the learners in the context of learning environments.
Typical solutions to integrate simulation models into learning environments are:

- Reprogramming of the simulation model
- Remodeling followed by an automatic code generation
- Remote access to the simulation model using a terminal client program
- Embedding the simulation model into a client/server architecture

The evaluation of the different solutions shows that the last one – integrating simulations within a distributed client/server architecture – is a very promising approach. It offers a tremendous variety of mechanisms to affect the simulation and its representation.
There exist some major demands for the use of simulation models within learning environments:

- User front end is embedded in the internet browser typically used by learning environments.
- A certain standard of quality can be assured for the simulation model integration.
- Different user interfaces and access levels for the author and learner are supported.
- Multi-user access at runtime and the individual administration of simulation runs are possible.

The client/server architecture can fulfil all these demands in a suitable manner. Embedding the simulation in a larger software system creates an additional layer which enables the simulation expert as well as the author to separate the model description from the input configuration and from the handling of the simulation results. On client side the middle tier layer is used to separate the server side calculation from the actual (and normally more simple) presentation of the results.
The basic concept of a self-contained model server architecture for a learning system is best described by the different roles and actors:

- Modeler: provides simulation models for the integration
- Author: integrates a simulation model into a specific learning environment
- Learner: uses the model without any context switch from within the learning environment
- System provider: provides and administrates the system and assures model quality

The practical example for integrating the Oxsoft Heart Program (which simulates the cardiac electrophysiology of the human heart) using a prototypical model server implementation as described above shows the feasibility of the concept in practice. Even if the prototype implementation fulfils the demands only rudimentarily at the moment, it can already be used in a real world medical learning environment with good success.

Architectural Concepts for Integrating Simulation components in Computer-Based Training Systems

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Abstract

Modeling and simulation of dynamic systems is an iterative process, consisting of model building and computer-assisted simulation by which the model structure and/or its parameters may be changed in an attempt to match the real dynamic system well. In fact the derived model has served its purpose when an optimal match is obtained between the simulation results and the data obtained from the real world system under test.

In general the model building process of a dynamic systems entails the utilization of several types of information sources which have to bear in mind:

- goals and purposes of modeling, determining boundaries, components of relevance, and the level of detail
- a priori knowledge of the dynamic system being modeled
- experimental data consisting of measurements on the dynamic system inputs and outputs
- estimations of non-measurable data as well as state space variables of real dynamic system

With respect to the spectrum of available models, a variety of levels of conceptual and mathematical representation is evident, which depends on the goals and purposes for which the model was intended, the extent of the a priori knowledge available, data gathered through experimentation and measurements on the real dynamic system or estimations.

With these basic considerations on modeling and simulation as a background, this paper analyses the relation between simulation software and the new type of software systems, the learning systems. As an overview in coupling web based training systems with simulation functionality, the several possibilities in architectural design for a –more or less- integrated system will be introduced at the very first. They may be summarized by four types of cases:

- no coupling
- loose coupling
- strong coupling
- full architectural integration by a method-based approach

These alternatives are explained and evaluated in detail. As a realization a project is introduced which considers well known knowledge from cognitive science, and allows the user to concentrate on engineering course materials without risk of becoming lost within the space of the multimedia educational network server. This topic is one of the most important to be considered, because with a user-adapted and consistently designed graphic user interface, the on-line working efficiency with the engineering educational material should increase in case of a good design and will decrease in the case of a less well or ill designed systems.

The paper ends with an introduction to one of the international standards in learning environment design: The LTSA is a high level systems architecture and layering for learning technology systems, known as learning technology, computer-based training, electronic performance support systems, computer assisted instruction, intelligent tutoring, education and training technology, and so on. The specification standard of this architecture is IEEE 1484 Learning Technology Standards Committee (LTSC) with subject areas: reference model, learner model standards, learning objects, task model, course sequencing, tools/agent communication, ontologies, data interchange, learning course management, different metadata categories, student, teacher, and tutor identifiers.

The concept for a flexible authoring and learning environment

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Abstract

This paper describes the concept for a flexible authoring and learning environment. It starts defining the requirements for the important flexibility of learning systems in respect to the current background of the learner, the dynamic ordering in which content is presented to the learner – also with consideration of the individual progress a learner makes – and the opportunity for the learner to proceed on many different paths in an exploratory way of learning.

To reach these demands a concept for a system architecture is proposed. The basic idea is to split the content into smaller units than usual, the so called 'content units'. Only doing so, the needed flexibility for individually adapted content, for an efficient handling of larger sets of content units, and the reusability for economic authoring can be assured.

On the other hand however, if the stored units get smaller than usual, a growing effort has to be spent to synthesize new content pages which are suited for the current learning situation and the current individual learner. It is the task to find approbiate content units which build a semantic senseful page unit. That is the reason why all relations between content units have to be explicitely stored by the system. This metadata set for each content unit includes technical information as well as semantical one. It splits in the parts

- technical information
- didactical information
- semantical information.

Following from this, the author has the task to provide these information for each content unit and to connect new content units to the already existing ones by reasonable relations. Afterwards the system has to evaluate the inter-related content units when a content page is asked by an user during his learning session.

The paper demonstrates the proceeding during the authoring and the learning phase by giving some details about the user classes with their roles and rights and by specifying those program modules which support the author in editing content units and in defining the relations between them. The following user classes are explained:

1. learning persons,
2. teachers,
3. authors,
4. system administrators,

To provide software support in managing the content units with their relations two program modules are necessary:

1. content unit designer:
   the content unit designer is an editor tailored especially to the demands of editing learning material for the learning system. It is based on a set of given templates and a given set of element types to fill the pages.
2. relation manager:
   The set of relations is extendable by the authors and thus can be individually adapted to cover special semantic restrictions and rules coming up from the context and/or background a content unit or even a complete course has. The specification and the administration of the relations is done graphically by linking graphically represented objects by labelled lines.

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Modelling and Control of Chemical and Bio-Chemical Processes

PRACTICAL ASPECTS OF SENSITIVITY ANALYSIS FOR DYNAMIC MODELS

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Sensitivity analysis studies the "sensitivity" of the outputs of a system to changes in the parameters, inputs or initial conditions which are often poorly known. Sensitivity analysis can be divided into two large categories: local and global sensitivity analysis. Local sensitivity analysis methods refer to small changes of parameters, while global methods refer to the effect of simultaneous, possibly orders-of-magnitude parameter changes. This paper will focus on local sensitivity analysis techniques. One of these sensitivity analysis techniques, the finite difference method, is discussed in detail and situated among other methods. The finite difference technique is often used to obtain a sensitivity measure, most of the time without considering the nonlinearity of the model or the round-off error introduced by the output calculations. These influences are analysed and discussed in detail.

The finite difference technique was implemented using a central difference formula.

$$\frac{\partial y_i}{\partial \theta_j} \approx \frac{y_i(t, \theta_j + \Delta\theta_j) - y_i(t, \theta_j - \Delta\theta_j)}{2\Delta\theta_j} \tag{1}$$

where $\Delta\theta_j$ is the change of the parameter value. Practically $\Delta\theta_j$ was implemented as the nominal parameter value θ_j multiplied by a user defined perturbation factor ξ. The choice of this perturbation factor will determine the quality of the sensitivity function. If the perturbation factor is taken too small it will result in numerical inaccuracies (figure 1). On the other hand, $\xi\theta_j$ should not become too large because then the nonlinearity of the model will start to play an important role in the sensitivity calculations (figure 2).
The advantage of using the central difference formula is that it can be used to assess the quality of the sensitivity analysis calculations using different criteria such as SSE (sum of squared errors), SAE (sum of absolute errors), MRE (maximum relative error) and RATIO (ratio between sensitivities). The error used in these criteria is the difference between the sensitivity functions calculated by perturbating the parameters up and down.

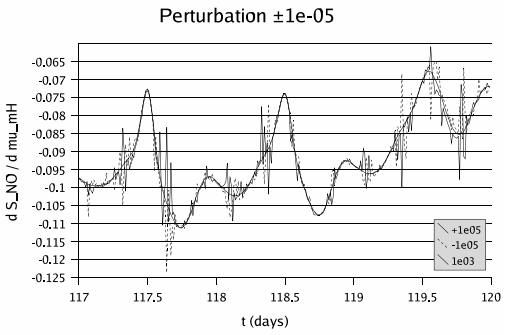

Figure 1: Effect of numerical error on the sensitivity function. Perturbation factor 10^{-5}.

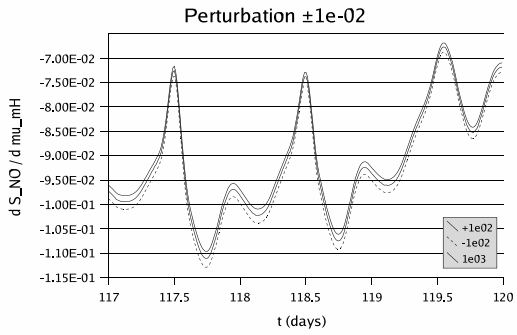

Figure 2: Effect of the nonlinearity of the model on the sensitivity function. Perturbation factor 10^{-2}.

The perturbation factor used in the finite difference method was found to be parameter dependent and to a lesser extent variable dependent. Among the proposed criteria the MRE and RATIO criterion were found useful to assess the quality of sensitivity function calculations. It was also found that the integrator accuracy has a large influence on the calculated sensitivity functions and the optimal perturbation factors.

Comparison of discretisation methods to solve a population balance model of activated sludge flocculation including aggregation and breakage

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A Population Balance Model (PBM) can be used to describe the time evolution of one or more property distributions of individuals of a population. This type of model was presented in the late seventies, but applications were limited due to a lack of computational power. Since the latter has significantly increased, the popularity of PBM increased which is reflected by an increase in the number of studies using this type of models. Applications can be found in different scientific areas dealing with a „population“ of individuals such as e.g. crystallization, flocculation, flotation, polymerization, precipitation,… The general format of a PBM looks like:

$$\frac{\partial}{\partial t} f(x,t) + \nabla_x \cdot \dot{X} f(x,t) = h(x,t) \qquad (1)$$

where x is a vector of properties, f(x,t) is the joint property distribution function, $\dot{X}$ is a vector containing the time derivatives of x and h(x,t) represents the birth and death of individuals typically occurring through aggregation and breakage (integral functions). In the application under study, activated sludge flocculation, the individuals are activated sludge flocs, the property vector x is chosen to be the floc size (one-dimensional PBM) expressed as volume and the distribution f(x,t) is chosen to be the number distribution. Growth is considered to be absent ($\dot{X} = 0$). Hence, eq 1 is of the integro-differential type and has no analytical solution. When discretising the property vector x, the integrals present in eq 1 (in h(x,t)) become summations and the integro–differential equation is converted into a set of ordinary differential equations that can be solved simultaneously using a time-integration algorithm. However, accurate solutions need a fine grid, which implies a high computational load. If one is interested in accurate estimates of certain properties of the distribution, other techniques can be used that were developed in order to decrease the computational load while still assuring the conservation of at least 2 integral properties of x (e.g. numbers and mass).

In this study, two of these techniques, the fixed pivot and the moving pivot, were used to solve the PBM using geometric grids ($v_{i+1}=s.v_i$, where v_i represents the floc volume and s>1). They were compared for three cases: pure aggregation, pure breakage and combined aggregation/breakage. In all cases total numbers and mass was conserved for all applied grids. For the pure aggregation case (Figure 1, left), it was found that the fixed pivot using a coarse grid overestimated the large particle sizes, since grid refinement produced a downward trend of the predictions. The moving pivot produced even lower predictions, but refinement resulted in an upward trend. The latter was, however, quantitatively much smaller and, hence, it can be concluded that the moving pivot is much closer to the pseudo-analytical solution even for coarse grids. For the pure breakage case (Figure 1, right), it was found that all moving pivot predictions and the fixed pivot for s=2 collapsed onto the same curve. The latter is due to the special type of breakage (binary into equally sized daughters). For other types of breakage, a similar behaviour as for pure aggregation will be observed (fixed pivot being worse than moving). Overall, it can be concluded that the moving pivot is superior over the fixed pivot since it produces more accurate predictions using coarser grids. The latter limits the computational load.

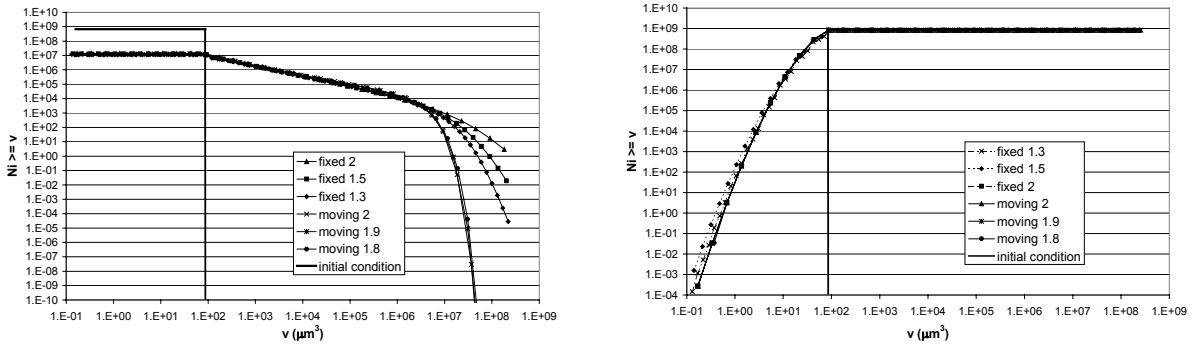

Figure 1 - *Comparison of fixed pivot and moving pivot for different grids: (left) pure aggregation, (right) pure breakage*

AN EXAMPLE OF THE BENEFITS OBTAINED FROM THE LONG TERM USE OF MATHEMATICAL MODELS IN WASTEWATER BIOLOGICAL TREATMENT

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Abstract

Anaerobic Digestion (AD) is a complex series of biological processes that take place in the absence of oxygen and by which organic matter is decomposed and bioconverted on one hand into biogas (*i.e.,* a mixture of mainly carbon dioxide and methane, a renewable energy source) and, on the other hand, into microbial biomass and residual organic matter. AD can be considered as one of the oldest and most efficient waste and wastewater treatment processes. It has been indeed applied over many decades for the treatment of household waste(water)s in septic tanks, of slurries in digesters, of sewage sludge in municipal treatment plants and of industrial wastewaters. It is also probably the major biological process involved in landfill wastes decomposition.

However, modeling of these processes is a tedious task that requires many efforts before obtaining satisfactory results. In addition, it is very difficult to find in the literature long-term evaluation of a model developed for AD processes.

This paper is concerned with a 0.947 m^3 anaerobic digestion fixed bed reactor used for the treatment of raw industrial wine processing wastewater. A mass balance model of this process was developed in 1997. This model was built to be simple but robust and thus only included two microbial populations (*i.e.,* acidogenic and methanogenic populations) degrading organic matter (expressed as chemical oxygen demand, COD) and producing volatile fatty acids (VFAs) and CO_2 in a first step, CO_2 and CH_4 in a second step.

The core of the present paper is to discuss the benefits of this five-year-old model from a practical point-of-view and the following points are highlighted:

- the model was demonstrated to be very robust and efficient over a very broad range of operating conditions (*i.e.,* COD in the output of the reactor between 0 and more than 10 g/l and total VFAs between 0 and 5 g/l) and over a large period of time (*i.e.,* five years after being developed and almost two years after a complete restart of the process – the reactor being then completely emptied and filled with new microbial populations),
- bad functioning of the overall process (*i.e.* a stop of a mixing pump at the bottom of the reactor that led to a working volume decreased by two thirds and a clogging of an important sensor, the pHmeter) could be discovered by comparison between on-line measurements and simulations of the model.

Acknowledgements

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Multiple steady state profiles in interconnected biological systems

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Based on a classical mono-biomass/mono-substrate mass balance model representation, an analysis of the multiplicity of steady state profiles in a cascade of bioreactors without backmixing for non-monotonic kinetic models is performed.
The first important issue of this work is related to the fact that such a configuration of bioreactor system is commonly used in biochemical engineering as well to simulate as to experimentally approximate the dynamical behavior of Piston-Flow Reactors (PFR). These processes exhibit very interesting properties such as a high reaction rate compared to the classical Continuous Stirred Tank Reactors (Cf. the pioneering work by (Grieves et al., 1964)). An immediate consequence is that the total volume of a PFR required to obtain a pre-specified conversion rate is smaller than the one required if a single CSTR is used. Being more appropriate to obtain high reaction rates- even in the case of an inhibitory effect of a high substrate concentration - PFRs are widely desirable in biochemical and biological engineering (including pharmaceutical and agro-industries). However, such systems are much more difficult to operate than CSTRs, in particular in transcient behaviors. Thus, if it is possible to obtain comparable - and in some cases even better - performances using a series of CSTRs instead of a single PFR, the associated industrial operation and reliability of such systems could be significantly improved.
Over the last twenty years, the fact that a series of CSTRs (Continuous Stirred Tank Reactors) could be used to approximate the behavior of a single PFR (Piston Flow Reactor) has motivated a large number of studies. In particular, the optimal design -where "optimal" has to be understood as the minimum total required volume to obtain a given conversion rate - of CSTRs in cascade has been investigated. Following this idea and using the mathematical optimization procedure proposed in [Luyben and Tramper,1982], [Hill and Robinson,1989] have shown that a cascade of only three perfectly mixed reactors with decreasing volumes could be used to significantly obtain the same input-output performances than a PFR for a comparable total volume. More recently, Harmand et al. have revisited the optimal design of two interconnected bioreactors for a larger class of kinetic models [Harmand et al., 2002].
However, none of these articles really investigated the structural properties of the system at steady state, such as the stability properties of the overall plant. In this work, the steady state properties of a series of N CSTRs are pointed out. Conditions under which a multiplicity of steady state profiles appears (depending in particular on the kinetic model and the number N of reactors in series) are explicitely derived for a class of non-monotonic kinetic models. The stability of these equilibria is also investigated using the Poincaré-Bendixon type results. Finally, it is shown that for sufficiently small volumes of CSTRs in series, it exists only one equilibrium, which is stable.

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Application of Experimental Designs for Modelling a Fermentative L-Valine Production Process by *Corynebacterium glutamicum*

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An iterative approach for model development using experimental design techniques is presented. The experimental design methods are used for either model discrimination or parameter estimation. For model discrimination, the criterion of Box and Hill [1] was extended for the discrimination between multivariate macrokinetic models using dynamic fed-batch experiments. In the iterative approach, the parameters of the models are re-estimated after each experiment using all available data. If none of the used models fit satisfactory to the data, the model structures need to be adjusted, introducing an increasing model complexity during the modelling process. If several (new) models fit satisfactory to the available data, a new model discriminating experiment can be designed. When only one satisfactory model is left, the next experiments can be designed in order to improve the estimation of the parameters of this model.

Here we report the first steps in the application of the experimental design method for the development of an unstructured macrokinetic model of an L-valine production process using a genetically modified strain of *Corynebacterium glutamicum*. A first set of models was made, based on qualitative analysis of a batch experiment and biological knowledge about the used strain. The models contained kinetic descriptions of the rates of biomass growth, glucose uptake, uptake of a second substrate and the production of L-valine. The second substrate is introduced because of the auxotrophy of the organism for L-isoleucine and pantothenic acid due to genetic modifications [2]. Several of the models could describe a simple batch experiment satisfactory.

Based on these results, a model discriminating fed-batch experiment could be designed. The best model so far did not describe auxotrophic behaviour with respect to the second substrate, in contrast to the other models. Therefore, experiment was designed with practically no supply of the second substrate so only this best model would predict any growth. This designed experiment has *not* been performed (yet).

Parallel to the modelling efforts, a fed-batch experiment was done aiming at producing high product concentrations and getting more information on the effect of the auxotrophies. After a first growth phase, glucose was fed into the reactor so that its concentration was kept at 3-5 g/l. No extra L-isoleucine or pantothenic acid were added. Surprisingly, the fed-batch experiment showed a steady ongoing growth for a long time after cessation of a short exponential growth phase. None of the first models were able to describe this behaviour properly. Therefore, the models had to be adjusted. Several of the new models fitted satisfactory to the fed-batch experiment, as illustrated by the figure alongside.

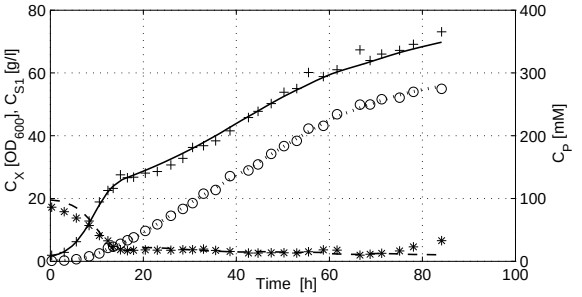

Figure 1: Fed-Batch Experiment: Measured concentrations of biomass (C_X) as +, glucose (C_{S1}) as o and L-valine (C_P) as *. Fitted model prediction of biomass as a solid line, glucose as dashed-, and L-valine as a dotted line.

Now, a new model discriminating fed-batch experiment will be planned again.

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MODELING OF THE METABOLISM DYNAMICS IN *ESCHERICHIA COLI* AFTER GLUCOSE PULSE EXPERIMENTS

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Mathematical models in biotechnology focus on the cellular metabolism as this may be exploited for the production of commercially important products. Metabolic models developed for the interpretation of pulse experiments can serve as a guide in identifying the main regulatory structures and provide quantitative information for the directed improvement of production strains.
In these transient experiments the intracellular metabolism of stationary grown cells is stimulated by a substrate pulse and the response of the key metabolites is measured with a high frequency (∼4-5 Hz). Due to the short sampling time of 30 - 40 seconds cellular processes, that require more time for action, like cell growth, cell division and genetic regulation can be neglected.
Models consisting of ordinary differential equations (ODEs) were built for the description of approximately 20 trajectories resulting from the experiments. Quantitative information about the enzymatic transformations necessary for the setup of the ODE system was retrieved from internet databases.
The parameter values of the enzyme kinetics were gained by fitting the models to the data.

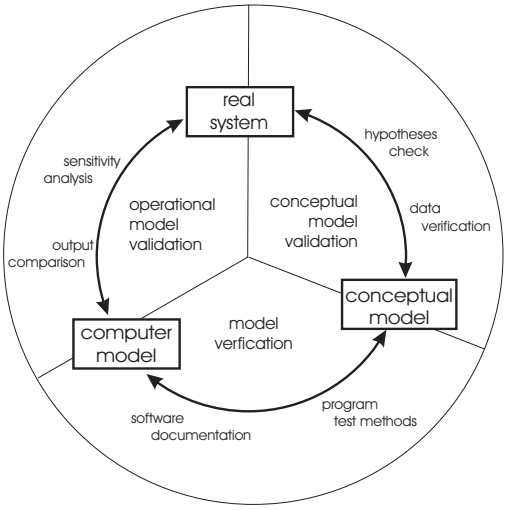

Fig. 1: Model building and validation process

Due its complexity the model building process could be subject to several sources of error, what leads to partial or total invalidity of the models. E.g. it could easily happen, that inadequate information is used for the setup of the ODE system, since different databases frequently contain contradictory information. That way several models could be found, that mirror the experimental data with a similar least square sum but make opposite prognoses. Another often mentioned problem concerning ODE models is the employment of redundant or artificial tuning parameters with intent to improve the results. Moreover inconsistencies within the data sets are possible due to the tedious procedure of the cell extraction and metabolite quantification.
So the models validity must be examined carefully, if the simulation experiments shall substitute laboratory experiments.

Some out of several tools, that were developed to prove the models validity at each step within the model building process (see Fig. 1, outer circle), will be presented.
A sensitivity analysis was performed with the aim to identify redundant parameters and groups of highly correlated parameters. Those parameters were eliminated from the models.
Statistical methods were applied to compare the modeling output functions with the experimental ones. E.g. the *bootstrap algorithm* was employed to check the model goodness for regression.
Due to the high data density an inductive modeling approach, the time series analysis, could be utilized to deduce the underlying reaction pathway from the experimental data sets. This modeling approach is completely independent from the described deductive approach and can be used for data verification, since the deduced information could be compared with a-priori knowledge of the system.

MODEL BASED OPTIMIZATION OF BIOCHEMICAL SYSTEMS USING MULTIPLE OBJECTIVES: A COMPARISON OF SEVERAL SOLUTION STRATEGIES

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Mathematical optimization provides a systematic framework to rationally design and/or operate biochemical systems. For many problems of interest one must find the best alternative for several (often conflicting) objectives. Thus, the real purpose of multiobjective optimization is to find the set of so called Pareto-optimal solutions set (i.e., the set of solutions that constitute the relatively best alternatives) which can then be readily used to choose suitable compromises for the optimal design and/or operation of the biochemical system. Very little has been done up to now regarding multiobjective optimization of biochemical systems. This is not surprising since this class of problems can be very challenging to solve, very especially due to the non-linear nature and potential non-convexity of these problems.

In this work, we consider the multiobjective optimization of ethanol production by *Saccharomyces cerevisiae*. The goals were to maximize ethanol production and simultaneously minimize several internal metabolite concentrations, imposing additional constraints in order to ensure cell viability. Starting from a mathematical model of the metabolic pathway available in the form of non-linear differential-algebraic equations, our main objective was to compare three recent solution strategies, highlighting the advantages and drawbacks of each one.

In the first strategy, we considered the solution of the non-linear multiobjective problem by means of the recent Normal-Boundary Intersection (NBI) method developed by Das and Dennis [1]. A second strategy used was the recent approach of Vera et al [3], Multiobjective Indirect Optimization Method (MIOM). Finally, in the third strategy, the problem was solved using the Multi-Objective Evolutionary Algorithm (MOEA) method of Tan et al [2].

Somewhat surprisingly, the MOEA method presented a rather poor performance (in terms of computational effort) when solving the case study. In contrast, the other two methods presented a good efficiency. From a biotechnological point of view, all methods arrived to somewhat similar results. It is possible to obtain different metabolic systems with an improved ethanol production while simultaneously minimizes intermediate concentrations. Also, multiobjective optimization can be a useful tool in the understanding of the factors that influence the metabolic flux. As an example, the figure shows the effect of two variables that were found to be critical in enhancing the ethanol production.

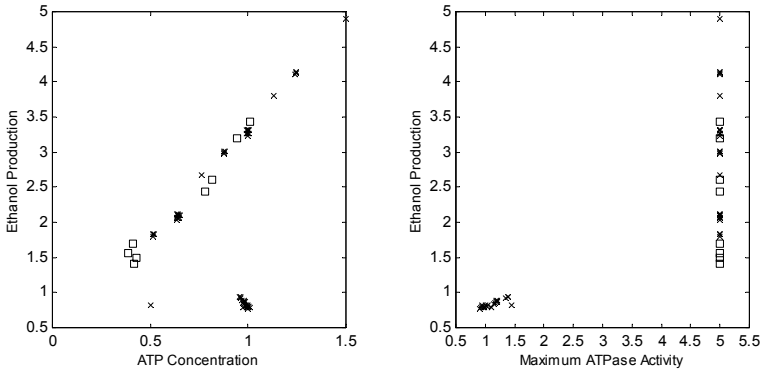

Figure 1. Effect of ATP and maximum ATPase activity in ethanol production. MIOM solutions (□). NBI solutions (**x**)

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ON ONE-DIMENSIONAL CONVECTION-DIFFUSION MODELS FOR SEDIMENTATION/THICKENING IN SECONDARY SETTLING TANKS

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The paper addresses the problems involved in the adequate modelling of sedimentation/thickening processes in secondary settling tanks of activated sludge wastewater treatment systems in the framework of one-dimensional conservation laws. We investigate initial boundary value problems for a convection-diffusion equation with a point source and a discontinuous convection field. We have first focused our attention on models with constant diffusion coefficient and demonstrated the strong dependence of the solution on the value of the diffusion coefficient. The specification of adequate boundary conditions, so far neglected in the literature, has shown to be of great importance. We emphasise the dependence of the diffusion coefficient on the flow field in the secondary settling tank, with the optimal closure being a function of turbulent viscosity; we have suggested a new closure with a spatially varying diffusion coefficient depending on the eddy viscosity of the fluid phase. We have performed a sensitivity analysis of the convection-diffusion models with the new closure with the use of turbulence measurements in a model secondary settling tank provided in the paper by Lyn and Rodi. The sensitivity of the convection-diffusion models with respect to the diffusion coefficient, and, therefore, the need of its recalibration with the use of turbulence/flow field measurements, are stated as the crucial points in the modelling of settling in the framework of one-dimensional conservation laws. A more rigorous analysis of the reproducibility of the diffusion coefficient requires, however, more extensive series of experimental data or multi-dimensional simulations of hydrodynamics in SSTs.

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MODELING BIOLOGICAL REACTION RATES USING RBF NETWORKS

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Over the past several years, neural networks (NNs), such as multilayer perceptron (MLP) or radial basis function (RBF) networks, have been increasingly applied to modeling and control of nonlinear dynamic processes.

NNs have long been used as black-box models, assuming no prior knowledge about the process, and entirely developed from sets of input-output data. NNs have proved to be powerful approximators of arbitrary nonlinear functions but, in turn, have strong requirements, in terms of quantity and quality, on the available experimental data. Indeed, both the structure and parameters of the NNs have to be inferred from this source of information.
In some application areas, e.g., chemical and biochemical processes, these requirements can be impossible to meet due to the lack of sensors and the fact that, when available, measurements are usually obtained at discrete times only, sometimes with relatively large delays, and are corrupted by noise.
To alleviate this difficulty, it is appealing to impose internal structure in the neural network model by incorporating available prior knowledge about the process [2]. Typically, this can be done by using first-principles, such as mass and energy balances, and by representing unknown terms or functions in the resulting mathematical expressions by NNs. This leads to the so-called serial approach. Alternatively, a parallel approach can be used, in which a first-principles model describing the process and a NN compensating for the modeling errors are connected in parallel.

The hybrid modeling approaches have several advantages:

- the model is by construction consistent with the underlying first principles;
- the size of the partial NN model and in turn, the number of unknown parameters, are reduced;
- parameter estimation requires less experimental data and leads to an optimization problem which is usually easier to solve.

In this paper, the serial and parallel hybrid approaches are applied to a real case study, e.g. batch CHO animal cell cultures, for which only rare and asynchronous measurements of a few macroscopic species are available.
Following the serial approach, two model structures are developed, in which RBFs are used to describe either the reaction kinetics or the complete reaction rates. In the former case, macroscopic reaction schemes are formulated, pseudo-stoichiometry coefficients are estimated independently of the kinetics, and a RBF model is derived for the specific reaction rates. In the latter case, pseudo-stoichiometry and kinetics are lumped together in a global RBF network.

Following the parallel approach, a first-principles model is first developed and the capability of a parallel RBF to compensate the prediction error of this model is investigated.

In the course of this study, special attention is paid to the several NN model identification steps, i.e., structural definition, parameter estimation (which is decomposed into unsupervised and supervised steps, the latter being in turn decomposed into linear and nonlinear optimization problems) and model validation. In this connection, several concepts are emphasized, including maximum-likelihood estimators, and the use of a weight decay procedure [1] to avoid identifiability problems.

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Dynamical Metabolic Modelling of Biological Processes

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Abstract

We are concerned in this paper with the identification of mathematical models of biological processes in the very common situation where measurements of extracellular species in the culture medium are the only available data besides measurements of the biomass itself. The aim of this paper is to investigate this question under a metabolic viewpoint. Therefore, as a starting point for our analysis, we assume that a metabolic network connecting the measured species is available. As a matter of illustration to our discussion we consider the example of CHO cells cultivated in batch mode in stirred flasks. The measured extracellular species are the two main substrates (glucose and glutamine) and the three most significantly released metabolites (lactate, NH_4, alanine).

The issue of bioprocess modelling from extracellular measurements has been considered for a long time in the literature. In classical macroscopic models the cells are just viewed as a catalyst for the conversion of substrates into products which is represented by a set of chemical "macro-reactions" that directly connect extracellular substrates and products without paying much attention to the intracellular behaviour. Dynamical mass balance models are then established on the basis of these macro-reactions by identifying appropriate kinetic models from the experimental data. During the last decade, a new trend in mathematical modelling has emerged by focusing on the so-called "Metabolic Flux Analysis", where intracellular fluxes are computed from the measured extracellular fluxes by using the stoichiometry of a metabolic network supposed to govern the system. Metabolic Flux Analysis is however essentially a steady-state analysis.

In this paper, our purpose is to throw a bridge between macroscopic dynamical modelling and metabolic flux analysis.

A "full modelling" approach could be considered. This means that we could try to find a global dynamical model which describes the full metabolic network, involving a separate state variable for each intracellular species and a separate kinetic model for each intracellular reaction. Such an approach, although conceivable, is in some sense "ill-posed" because the intracellular kinetics are in general not structurally identifiable without intracellular measurements. We shall rather follow a "reduced modelling" approach where the model is based on a set of macro-reactions which are compatible with the underlying metabolic network and supported by a preliminary metabolic flux analysis.

The model development proceeds in three steps. First we perform a metabolic flux analysis in order to check the consistency of the assumed metabolic network with the experimental data. In a second step, we compute the elementary flux modes of the metabolic network which are readily translated into a set of elementary macro-reactions connecting the extracellular substrates and products. Finally, in a third step, a classical dynamical model is established on the basis of the macro-reactions. An interesting consequence of this modelling approach is to allow the prediction of the time evolution of end-products which are not measured. The procedure will be presented through the case study of CHO-320 cells cultivated in serum free medium.

BIOSORPTION OF PYRENE TO PHOSPHOLIPID MEMBRANES – A MOLECULAR DYNAMICS STUDY

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Polycyclic aromatic hydrocarbons (PAH) are toxic, carcinogenic and mutagenic organic pollutants. They are produced by partly combustion of organic matters such as fuel or wood. With the rain they are introduced into rivers, lakes and sewage water. Due to their hydrophobic nature they are hardly soluble in water. They adsorb at hydrophobic compounds in the environment, such as dust particles, soil particles or organisms. PAH diffuse passively into micro-organisms. Most of the micro-organisms cannot degrade PAH. After diffusing into the cell membrane the PAH are immobilised there. This means on the one hand that an uptake of PAH by higher organisms is prevented. On the other hand they are not available any more for further degradation. Thus the residence time in the environment increases. Several works exist which are dealing with the sorption and decomposition of PAH but they are mainly investigating on macroscopic scale, such as balance models [1], [2]. Processes on microscopic, atomic scale are not taken into account. With molecular dynamic simulations it is possible to get an access to sorption and diffusion processes on atomic scale. Thus prediction of the effects caused by accumulation of PAH on the physical and physiological properties of the lipid membrane is possible.
A molecular dynamic simulations is presented to characterise the behaviour of polycyclic aromatic hydrocarbons in phospholipid bilayers. As model substance of PAH the flat molecule pyrene was chosen. The molecule consists of four condensed benzene molecules. A fully solvated oleoyl-palmitoyl-sn-glycero-phosphocholine (POPC) bilayer serves as model membrane [3]. The diffusional motion of pyrene into and inside lipid membranes was simulated over a span of 10ns. The simulation was carried out with Gromacs 3.0 [4] package on two dual processor PC.
Despite the starting position of the pyrene molecules after a few nanoseconds all molecules had moved to z-position in the membrane which is located about 1.0 to 1.2nm away from the phosphorous atom of the head groups. No further movement in z-direction is detected afterward. From trajectories file it can be seen that the movement in x- and y- direction is not affected. This indicates the existence of a transport barrier through the lipid membrane.
The rotation of the flat molecule pyrene round the molecule's long axis and the orientation toward the z-axis of the membrane were calculated. The pyrene molecules inside the membrane can rotate freely around its long axis but show a strict orientation towards the z-axis. It does not exclude a temporary rotation or bending to one or the other side but this movement seems to be restricted.
The thickness of membrane is contemplated as thickness between the oxygen atoms of the glycerol group (arbitrary choice). The distance is the average distance between all the oxygen atoms of one half of the membrane and the other half of the membrane. By comparison of the distance calculated from the simulation with pyrene and a simulation without pyrene no membrane swelling can be detected.

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Model Simplification and Model Reduction

ORDER REDUCTION FOR SECOND ORDER SYSTEMS

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Components of microsystems can often be described by partial differential equations (PDE). The semi-discretization of these PDEs usually leads to large systems of ordinary differential equations (ODE) of the form

$$\boldsymbol{M}\ddot{\boldsymbol{x}} + \boldsymbol{D}\dot{\boldsymbol{x}} + \boldsymbol{K}\boldsymbol{x} = \boldsymbol{B}\boldsymbol{u} \quad (1)$$

$$\boldsymbol{x}_a = \boldsymbol{B}_a^{\mathsf{T}}\boldsymbol{x} \quad (2)$$

with $\boldsymbol{x}(t) \in \mathbb{R}^N$, $\boldsymbol{M}, \boldsymbol{D}, \boldsymbol{K} \in \mathbb{R}^{N\times N}$, $\boldsymbol{B} \in \mathbb{R}^{N\times m}$, $\boldsymbol{u}(t) \in \mathbb{R}^m$, $\boldsymbol{B}_a \in \mathbb{R}^{N\times p}$. N can be large ($10^3 \ldots 10^5 \ldots$). Often, $\boldsymbol{M}$, $\boldsymbol{D}$, and $\boldsymbol{K}$ are symmetric and positive semidefinite.
The interpretation of the matrices depends on the application. For mechanical systems, $\boldsymbol{M}$, $\boldsymbol{D}$, and $\boldsymbol{K}$ are the mass, damping and stiffness matrices. $\boldsymbol{B}$ is the (generalized) incidence matrix of points with applied forces, thermal input, currents etc., $\boldsymbol{u}$. $\boldsymbol{x}$ is the vector of displacements, temperatures, voltages, currents etc. $\boldsymbol{B}_a$ is the (generalized) incidence matrix of active nodes or observation points $\boldsymbol{x}_a$. Often, especially for components in system simulation, the terminals are at the same time the observation points, $\boldsymbol{B} = \boldsymbol{B}_a$.
Due to constraints on computational time and memory when using these models of components in system simulation, the large systems (1,2) are approximated by systems of considerably lower dimension,

$$\tilde{\boldsymbol{M}}\ddot{\tilde{\boldsymbol{x}}} + \tilde{\boldsymbol{D}}\dot{\tilde{\boldsymbol{x}}} + \tilde{\boldsymbol{K}}\tilde{\boldsymbol{x}} = \tilde{\boldsymbol{B}}\boldsymbol{u} \quad (3)$$

$$\boldsymbol{x}_a = \tilde{\boldsymbol{B}}_a^{\mathsf{T}}\tilde{\boldsymbol{x}} \quad (4)$$

with $\tilde{\boldsymbol{M}}, \tilde{\boldsymbol{D}}, \tilde{\boldsymbol{K}} \in \mathbb{R}^{n\times n}$, $\tilde{\boldsymbol{B}} \in \mathbb{R}^{n\times m}$, $\tilde{\boldsymbol{B}}_a \in \mathbb{R}^{n\times p}$, $\tilde{\boldsymbol{x}} \in \mathbb{R}^n$ and $n \ll N$, usually $n = 10 \ldots 100$. This is called order reduction.
During the 1990s projection methods became a popular and powerful tool for order reduction. Here a first order system ($\boldsymbol{M} = 0$ in (1)) is projected into Krylov subspaces of $\mathbb{R}^N$ by a Lanczos or Arnoldi algorithm [1]. To use these methods for second order systems (1), they have to be transformed into a first order system which means doubling of the system dimension and loss of symmetry and definiteness properties. In 1999 the ENOR algorithm was developed for RLC circuits which is well adapted for second order systems [2].
The algorithm presented in this article is based on ENOR but has some improvements. After Laplace transformation into frequency domain the system can be expanded about the Laplace variable $s_0 = 0$ which ensures an exact solution for the static case. Furthermore, the system can be expanded at several points in the frequency domain simultaneously, so the original system is well approximated in the frequency domain and in the time domain.
Examples from several domains demonstrate the power of our algorithm. For instance, an acceleration sensor could be reduced from $N = 18102$ to $n = 6$ with very good accuracy.

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Positive Real Reduction : an LMI-based Algorithm

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This paper is based on some simple remarks concerning the *Hankel* norm approximation. A remarquable property of this approximating technique is that it gives bounds on the error. Considering the classical state-space formulation of a linear system Σ, we have :

$$\sum \left\{ \begin{array}{l} \dot{x}(t) = Ax(t) + Bu(t),\ x(t_0) = x_0 \\ y(t) = Cx(t) + Du(t) \end{array} \right. , \tag{1}$$

where $x \in X \subset \mathbb{R}^n$ is the state, $x_0 \in X$ is the initial state, $u \in U \subset \mathbb{R}^m$ is the input and $y \in Y \subset \mathbb{R}^m$ is the output.
The gamians of Σ are defined as the solutions of the following *Lyapunov* equations

$$\left\{ \begin{array}{l} AG_B + G_B A^T + BB^T = 0 \\ A^T G_C + G_C A + C^T C = 0 \end{array} \right. , \tag{2}$$

where G_B is the observability gramian and G_C is the controllability gramian.
The singular values of Σ are defined as the square-root of the eigenvalues of $G_B G_C$.
If ϵ denotes the *Hankel* norm error, from [1] we have :

$$\sigma_{k+1} \leq \epsilon \leq \sum_{i=k+1}^{n} \sigma_i \tag{3}$$

where σ_j is the j^{th} ordered singular value of Σ.
It is clear from (3) that the error is optimal only if $k = n - 1$. On the other hand we can try to improve the error for $k < n - 1$. In [2,3], *Anders Helmersson* suggests a convex optimisation formulation of this problem by means of *LMIs* (Linear Matrix Inequalities) [4]. By doing this he obtains an efficient algorithm to approach the optimal Hankel norm approximation error. It must be kept in mind that such a technique cannot be applied to high order systems. It works well only with systems with a state with a few tens of components. Although the error diminution is marginal, a few percents (in the exemples of [2,3] it varies from $2,6\%$ to $7,5\%$), it could be of great relevance in cost terms.
Here our goal is to derive new algorithms, based on the ideas of [2,3], which objective is of a different nature. The Hankel norm approximation is useless in our approach. Given a pair of passive reduced-order models (of different orders) we want to reduce the distance between them measured by means of the H_∞ norm of their transfert function difference. This optimisation has to be done with passivity preservation. This could be important because of practical implementation considerations or to keep coherent the energy behaviour of the reduced-order model in its environment with respect to the original model.

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A Simulation Free Nonlinear Model Order Reduction Approach and Comparison Study

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The simulation, analysis and controller design of nonlinear control systems are complicated. These tasks can be simplified by reducing the order of the original system and approximate it by a lower order model. In this paper a new approach to the model order reduction of nonlinear systems is presented. This approach does not need simulation of the original system and therefore it is suitable for large systems.
By separating linear and nonlinear parts of the original nonlinear model, the idea is considering the nonlinearity of the system as additional inputs. So, without loss of generality, a nonlinear system of the following form is considered,

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \underbrace{\begin{bmatrix} \mathbf{B} & \mathbf{F} \end{bmatrix}}_{\mathbf{B}^*} \underbrace{\begin{bmatrix} \mathbf{u} \\ \mathbf{g}(\mathbf{x},\mathbf{u}) \end{bmatrix}}_{\mathbf{u}^*}. \tag{1}$$

The vector $\mathbf{g}(\mathbf{x},\mathbf{u})$ exclusively comprises the *nonlinear* parts of the system that is, every such term appears only once and is free from any possible constant factors. Now, we consider $\mathbf{u}^*$ as a new input of the system. This linear system can be reduced using a known linear order reduction method like the one described in [1] and the matrices $\mathbf{A}_r$ and $\mathbf{B}_r^*$ are computed. An approximation of the original states is constructed as a linear combination of the states and inputs of the reduced order system which is used to reconstruct the original states and the vector of nonlinearities which requires the full state vector. The reduced order model is then

$$\dot{\mathbf{x}}_r(t) = \mathbf{A}_r\mathbf{x}_r(t) + \mathbf{B}_r\mathbf{u}(t) + \mathbf{F}_r\mathbf{g}(\mathbf{W}\begin{bmatrix} \mathbf{x}_r(t) \\ \mathbf{u}(t) \end{bmatrix}, \mathbf{u}). \tag{2}$$

For comparison to some known methods in order reduction of nonlinear systems, three other methods are discussed briefly:

1. Proper orthogonal decomposition which uses some simulation results of the original system and put them at some sampling points in a matrix called snapshot matrix. By performing a singular value decomposition (SVD) of the snapshot matrix and finding a projection using an approximation of the original states from reduced states, the reduced model is found.

2. Optimizing the system matrices [2] in which some simulations of the original system is performed and the results at some sampling points are combined into snapshot matrices. By minimizing some errors, a reduced order model of the type (2) can be calculated by an explicit formula.

3. Using projection from linearized model which finds a projection matrices from analyzing a linear model, typically a linearization of original nonlinear model at some operating points and then applies the projection to the original nonlinear model.

At the end, a hydro pneumatic vehicle suspension is considered [2]. The original system has 10 states, 2 inputs and 5 nonlinearities ($\mathbf{F} \in \mathbb{R}^{10\times5}$). All of the four methods were tried to be applied to this system. Because of using limiter and sign function in the system, linearization is not possible and linearized model can only be found by neglecting some important parts. Therefore, other three methods were successfully applied to the system. The system is reduced to order 6 and the results are compared and discussed.

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Generation of Linear Models using Simulation Results

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Abstract: In many applications very fast models of as low order as possible are required. In the last time powerful methods have been known which are used for the order reduction of high dimensional models. Basing on the knowledge of the matrices $\Sigma = (A, B, C, D)$ of the high dimensional model these methods determine a suitable subspace and project transient processes of the system into this subspace. On the powerful methods the subspace is determined using balanced truncation or as a Krylow-subspace, respectively.
If the matrices $\Sigma = (A, B, C, D)$ are not available these methods cannot be used.
This is the case if a simulation model is available, but it is not possible to extract the matrices of the system. If the simulation model is large, the simulation slow and one needs much simulation runs, one looks for a simplified fast model of as low order as possible.
In the paper a two step approach for the generation of linear models using impulse response values which are computed by simulation will be described. In the first step a model of a "middle" order is determined using a realization based method. In the second step the order of this model will be reduced using known model order reduction methods. The objective of the paper is to show, that this kind of modeling realized by a combination of well known methods works reliable and leads to accurate models of very low order.
The determination of a model from given step or impulse responses is like an identification task. But the use of classic identification approaches like PEM or IVM is unfavorable. These identification methods are developed for the determination of models from experimental data, i.e. disturbed measurements. They are specialized for the handling of disturbances in the process output which occur in all real measurements. But if there is a high number of inputs and outputs or a high systems order their numerical properties are very poor. In the case of nearly undisturbed data like simulation results these methods are without advantage.
Recently developed subspace methods have better numerical properties. Optimization steps are not needed. The multi-input multi-output case can be handled in the same way as the single-input single-output one. Initial values are not needed. An important advantage in practice is the simple determination of the model structure by only one parameter, the model order. If it is possible to determine the step-response or impulse response directly, simplified (basic-) versions of these methods can be used. These are much more robust and their application can be extended to large systems. We propose the usage of an approach, close related to the realization framework. From the Hankel matrix, assembled by impulse response values, a partial realization will be determined, using the singular value decomposition. This approach yields models which are very accurate in the starting sector of the impulse response. But the static behavior is not so good. To obtain models with small static errors often the partial realization has to be of relative high ("middle") order. In such cases it will be suggested to reduce the order of the analytic "middle" order model in a second step with known standard methods like modal or balanced truncation, with or without singular perturbation, respectively.
The application of the two step approach is demonstrated by three examples. The first example "gasf" from the MATLAB Control System Toolbox demonstrates the capability of the first step, to handle magnitudes of great differences (static factors from 10^{-5} to 10^{+5}) between amplifications of different input-output branches. In the second example the temperature distribution of an analog amplifier-IC will be considered. The original FEM model consists of 27.956 nodes. The temperature distribution caused by the heat power of the output stages is computed in 102 locations. By the first step one gets a good model of order 21, by the second step the order can be reduced to 15. The third example is an micro system acceleration sensor. The original FEM model is of order 16095. The first step yields a model of order 8. The model order can be reduced to a second order system. In the time domain no differences between the original and these two models are visible. The Bode plot shows differences at very high frequencies.
The conclusion of the paper is: the combination of well known approaches to

- calculate a partial realization via factorization of the Hankel matrix using svd and
- model order reduction by modal or balanced truncation

yields a powerful and fast tool to generate time discrete state space models from given impulse response values. The two-step approach yields in most applications significantly better results than the modeling of the low order already in the first step. The method works well on large systems too. The models are accurate and of very low order.

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On the Modelling, Simulation and Control of Mobile Systems

EMBEDDED MICROCONTROLLER DEVELOPMENT PROCESS WITH APPLICATION TO SELF-LEVELING STABILIZED PLATFORM

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When sophisticated system theories are correctly and successfully applied to control complex systems behavior, the resulting performance can be very impressive. This paper presents such a case study in designing and synthesizing an embedded microcontroller that implements a sophisticated estimation and control algorithm for a self-leveling and stabilized platform, which is shown in Figure 1. The control objective is to self-level the top platform and stabilize its motion, in spite of disturbance caused by motion of the base platform.

This paper describes a ***"near-zero hand-coding" (NZHC)*** hardware and software development environment and process for programming an embedded microcontroller. The NZHC process begins with math modeling of the systems to be controlled. **Matlab./Simulink** simulation and **VRML** (virtual reality modeling language) visualization of the system performance not only provide approximate numerical results, but more importantly reveal insights to the overall scheme. State-of-the-art auto-coding software tools, such as **MakeApp** and **TargetLink**, allow a user to use graphical user interface (GUI) and generate C-source codes from selected functions and Simulink simulation block diagrams. **Hitachi WorkBench** software is then used to combine the C-source codes into a main program.

The environment was used to develop a **Hitachi SH2 Evaluation Board** microcontroller that implements a Kalman estimator and PID controller for self-leveling and stabilizing a platform. The microcontroller was also used to communicate with a Simulink on PC for monitoring performance of the controlled system. The turn around time for code compilation, download and test is approximately 30 seconds, which is very useful for calibration and gaining practical insights on the system being control.

Figure 1 also shows the hardware/software development setup for self-leveling stabilized platform experiment, using an embedded Hitachi SH2 Microcontroller to implement the designed filters and controllers. The SH2 is a powerful 40MHz floating point processor with a large array of I/Os, including A/D, D/A, DI/O, PWM, counter and clock modules, and an extensive set of instructions. A Kalman filtering technique is used to fuse complementary information from MEMS (Micro-Electro-Mechanical-System) tilt sensors (accelerometers) and angular rate sensors. Proportional-Integral-Derivative (PID) controllers are applied to drive the actuators (dc motors) and balance the platform.

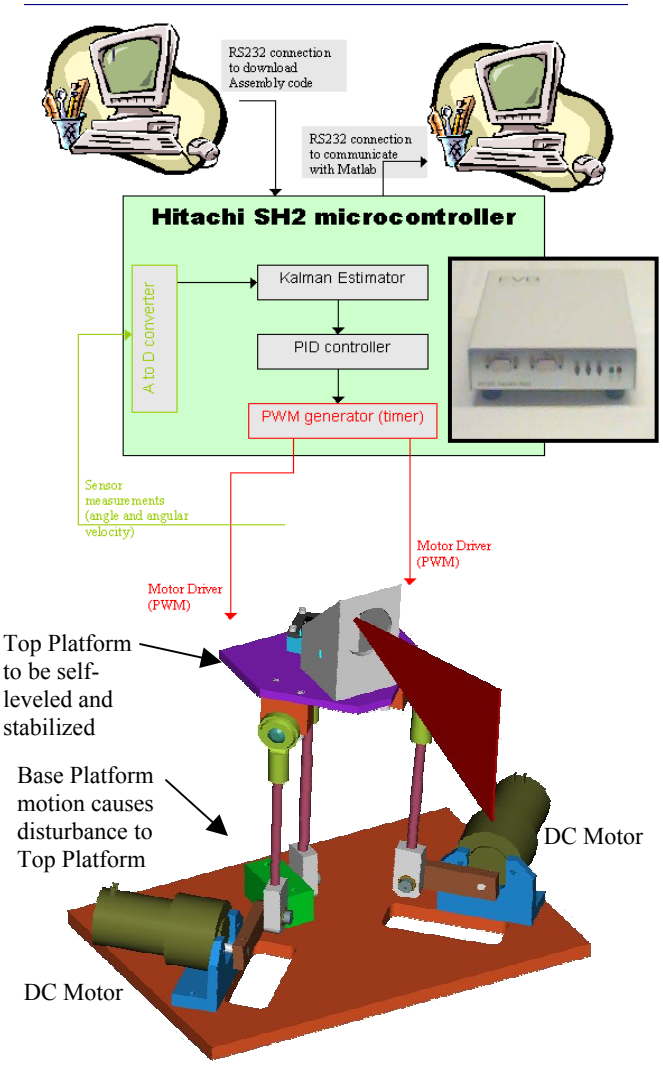

Figure 1. Hardware/Software Development Setup for Self-Leveling Stabilized Platform System Experiment with Embedded SH2 Microcontroller

Modeling and Reduction Techniques for Studies of Integrated Hybrid Vehicle Systems

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Vehicle development is a costly and time consuming process: it begins with a comprehensive analysis of the vehicle to determine the desired characteristics of its systems, it proceeds with the detailed design of systems, subsystems, and components, and it concludes with the building and testing of prototypes. The latter may include engine, drivetrain, or vehicle subsystems and components, as well as the complete vehicle. In the case of hybrid powertrain vehicles, this process becomes even more cumbersome and time consuming due to the complexity of the systems and the increased number of subsystems and components. Development time and cost can be significantly reduced through the use of modeling and simulation. Modeling by means of time-based simulations allows the testing of virtual vehicles for a variety of conditions, and designing of subsystems and components at the early stages of development. In addition, a model-based simulation assists in quantifying parameters associated with subjective driver feel and overall drivability that are difficult to measure and yet very important for customer acceptance. However, the effectiveness of modeling and simulation is heavily dependent on the availability of comprehensive vehicle system, subsystem, and component models of appropriate fidelity. A simple yet accurate dynamic model (proper complexity model) of the integrated vehicle can generate vehicle responses in a short time while including only the important physical phenomena based on the variables of interest. These proper complexity models can then be used for efficient simulation-based design optimizations. This work presents the development and reduction of a bond graph-based integrated hybrid vehicle model to the proper level of complexity. This model will be later used for optimizing fuel economy while maintaining critical performance characteristics. Therefore, a model that accurately predicts performance and fuel economy variables is necessary. The vehicle is composed of the engine, drivetrain, and vehicle dynamics systems. In addition to the conventional powertrain, a hybrid propulsion system is included, consisting of a hydraulic propulsion and energy storage subsystems. Model reduction methodologies (energy-based modeling metrics) are employed to identify the critical system parameters and reduce the model size, while providing more insight into the system. They also generate more computationally efficient models. In addition, the vehicle dynamics system is reformulated into explicit equations to further improve the efficiency of numerical integration. A military truck that belongs to the Family of Medium Tactical Vehicles (FMTV) is selected for the implementation of the modeling and reduction procedure. A realistic speed cycle and a road profile representative of the FMTV mission are used for the evaluation of the energy-based modeling metric. The reduced model of the hybrid FMTV truck is obtained in a short time using this systematic modeling procedure. The reduced model accurately predicts all variables of interest (e.g., fuel consumption in Figure 1) and requires 2.5 times less time to calculate the vehicle response. Simulation-based design optimization can then be performed to obtain an optimal design by means of the computationally efficient truck model. The design optimization procedure is beyond the scope of this paper and is presented in Filipi et al. [1].

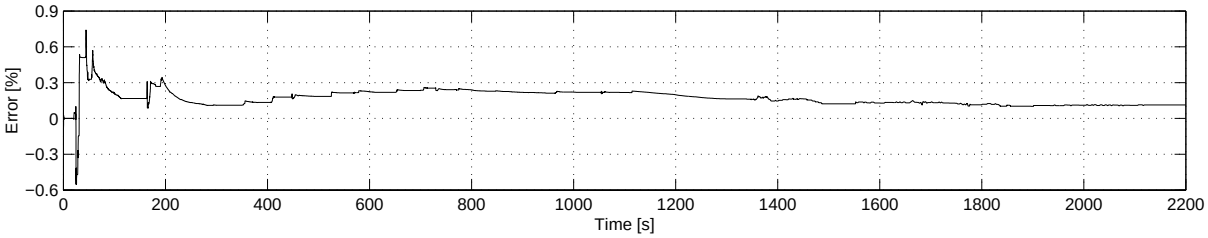

Figure 1: Fuel consumption accuracy (full vs. reduced model)

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EVALUATION OF ADVANCED SHORT-RANGE RADAR TRACKING ALGORITHM

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Available statistics on motor vehicle traffic crashes in the United States shows alarming fatality and huge associated costs. For example, in 2000, there were 42,000 fatalities from 6.394 million police-reported motor vehicle crashes; 3.2 million people injured, and 4.3 million crashes with property damage only; approximately $200 billion of economic cost resulting from motor vehicle crashes. Automobile active safety systems, including collision warning, avoidance and impact reduction systems, are being researched extensively by automobile manufacturers and their first-tier suppliers. The premise of the effort is that the needed systems can be developed with today's technologies, to help save lives, minimize crash impact and injuries, and/or prevent accidents from occurring.

One of the active safety schemes being investigated is the use of short-range radars (range up to 20 meters) to warn drivers of potential collision situation that may arise unexpectedly. Figure 1 shows an experimental hardware setup where four short-range radars are mounted on the bumper of an SUV. The objective is to fuse the information from these radars and track objects in the traffic in the view of the radars. The major concerns in such a scheme are to correctly track bona fide objects and accurately predict their motion, while precluding false alarms. Figure 2 shows a configuration of the off-line and real-time online software development techniques that the authors are employing to evaluate algorithms for monitoring traffic from the radar setup.

This paper describes the hardware and software techniques to conduct experiments with the short-range data. Algorithms for processing noisy and misleading radar information will be shown. The software entails appropriate use of fuzzy logic, fuzzy clustering, neural networks and Kalman filtering. Results from the study will be shown.

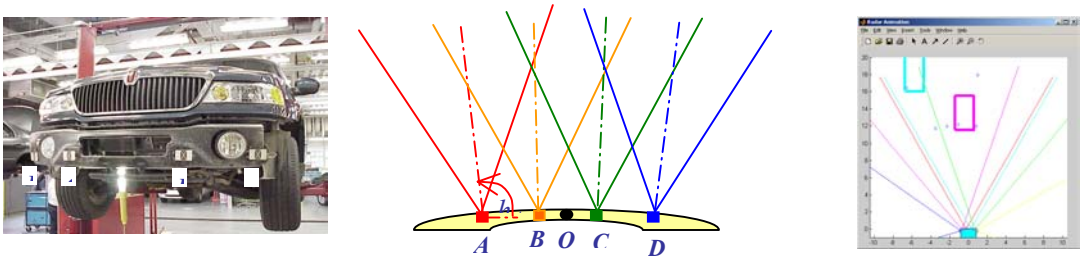

Figure 1. Experimental setup of Short Range Radars on a Ford Lincoln Navigator

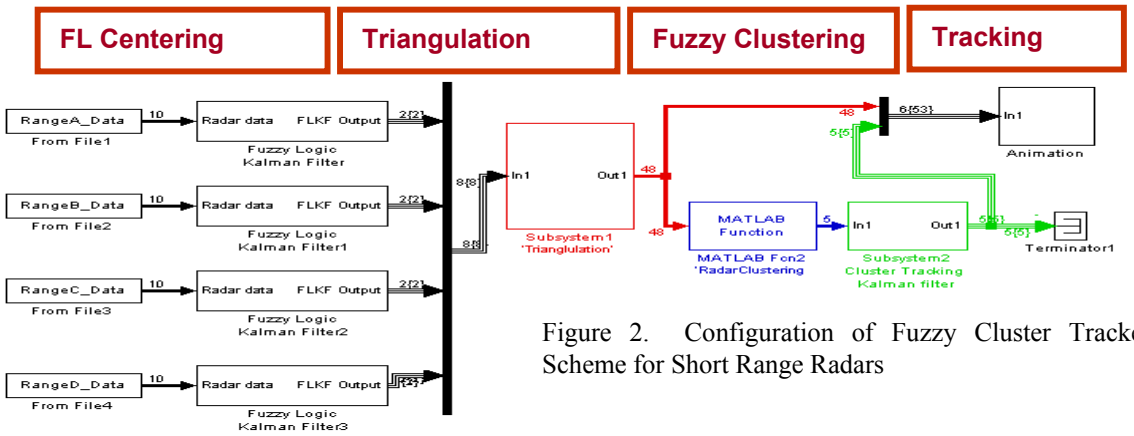

Figure 2. Configuration of Fuzzy Cluster Tracker Scheme for Short Range Radars

24 DEGREES-OF-FREEDOM VEHICLE DYNAMICS MODELING FOR MULTI-CPU DRIVING SIMULATION ENVIRONMENT

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The introduction of Simulation techniques in the early design and development process for the purpose of function verification and performance evaluation has caused tremendous improvement in cost reduction and time-to-market for the automotive industry.

Full-vehicle driving simulations are one of these kind of applications. Vehicle simulators often remain inaccessible for customization or alternate applications with external workstations. For example, numerous vehicle simulation packages are commercially available (e.g. Adams, DADS, Truck-SIM, STI). All of these packages allow for configuring the parameters of the mathematical structure of the vehicle model, and not for alternating the model itself.

Oakland University has developed a driving simulation environment for which the mathematical architecture is completely accessible and re-configurable using external workstations. This allows the vehicle model to be modified and adjusted to virtually any human-in-the-loop driving simulation application. Additionally, the interfacing with the architecture has been developed in Matlab/Simulink, and therefore provides for an easy-to-use design environment. The work stations are connected in a fast local area network, generally available in academic and industry environments.

The key this new architecture is the use of a re-directional vector table, which is used to index the values of the state vector. The mathematical formulation of any dynamic model can be represented by a state space formulation. The transition matrix defined the derivation of each of the states from the other states. By alternating the vector table, one of the state values can be redefined in another model. In other words, one of the rows of the transition matrix can be replaced without loss of generality for the overall system model. When this method is applied to a particular set of state values, then the sub-model of the vehicle which is represented by these states can be replaced with another model, for example a passive suspension system can be replaced with an active suspension system.

The implementation of this vector table architecture through a communication network redefines how the model is solved for each integration step during the simulation. For real-time simulation, we are limited in the use of integration methods that we can use. Unfortunately the vector table architecture inherently forces the solver to execute forward Euler integration, which is less accurate and less stable than more sophisticated methods.

This paper describes the mathematical and algorithmic architecture of the driving simulation environment and the implications for executing the simulation with the human-in-the-loop. We will also discuss options for improving performance and accuracy by adjusting integration methods.

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Physical Modular Modelling and Simulation

VirtMould – a framework for simulating component-oriented models of mechatronic systems

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We present here the main features of `VirtMould`, a software that provides tools and interfaces dedicated to modelling and simulation of complex engineering systems. Developed in the frame of the project `VirtMould`, supported by institute RISC of Johanner Kepler University, Linz and company Engel from Schwertberg, Austria, the software was meant to produce models of injection-moulding machines, on which software developers from Engel could run and test programs for the PLC embedded in the moulding machines.

From the mathematical point of view, the most important part of our software is a compiler for a modelling language. For developing the models, we used `Modelica`, a new high-level language, dedicated to object-oriented multi-domain modelling of physical and engineering systems. `VirtMould` integrates a compiler for a subset of this language; we focus in our paper on features of this compiler.

`Modelica` (see `Modelica` tutorial [1] and specifications [2]) allows high level modelling by composition of components; on the other hand, detailed models of components can be created, using the describing equations. An important feature is that it allows *discontinuous variables*; the discontinuities are handled by generating events.

Currently there exists one compiler for the standard specifications of `Modelica`, provided by Dynasim (Sweden) as part of the `Modelica` simulation environment Dymola. After studying the features of this compiler against the necessities of our project, the designers of `VirtMould` decided to provide a different compiler for `Modelica`. Initially, only block-oriented models have been supported (the components had a clear structure of inputs and outputs). A later version supports non-causal modelling.

In multi-domain non-causal modelling, non-trivial application tend to have mathematical descriptions expressed as very complex implicit systems of differential and algebraic equations, whose sizes range up to hundreds of thousands. We ease the burden of numerical solvers by preserving the *granularity* of the models as much as possible. More exactly, the compiler tries to bundle the equation within the component of lowest structural complexity, which has a definite structure of inputs and outputs. In this way, instead of passing a huge system of equations to numerical solvers and integrators, a number of systems of reasonable sizes are sent.

After compiling the initial `Modelica` text, a *dynamic-link library* is generated. This library encapsulates both the model description and the integration algorithms. Among the possible services provided by this library we mention starting/stopping a simulation process, and transmitting the names and values of all the internal variables of the model, at every time moment during the simulation run.

In order to interact with other programs, we used a common interface built upon the COM (*Common Object Model*) technique. A COM interface component for loading and unloading simulations, calculating time steps and exchanging data with the simulation has been designed.

For visualizing the results of the simulation an OPC (*Object linking and embedding for Process Control*) server has been developed and implemented. The simulation results are provided via OPC and these values can be visualized with standard OPC client tools.

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Development and Application of the Modelica Library TechThermo

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The increasing demand for analyzing dynamic systems has encouraged the development of new simulation tools. The general purpose simulation language Modelica [1,2] has been developed to improve the efficiency of the modeling process by applying object-oriented techniques. The availability of model libraries containing the base modules needed to build a system is essential for the economic application of Modelica. Different libraries are already available. The Modelica library TechThermo provides descriptions for components needed in systems including thermodynamic processes. TechThermo is intented for engineering applications without being restricted to a certain thermodynamic application.

This library should enhance the efficiency by providing definitions for interfaces. The experienced user can create problem-specific models by extending models from TechThermo thus shortening the development time. The models provided by TechThermo should allow a quick analysis of simple transient systems with only minor additional modeling effort. A detailed analyis demands the implementation of problem-specific models. Although it would be comfortable to have an universal thermodynamic library which allows the modeling of any system by combination of basic models without input of further model equations, the implementation of such a library seems not to be feasible in practice Instead, the aim of TechThermo is to minimize the effort for supplementary models for a wide range of application.

This paper describes the characteristic demands resulting from simulations of transient thermodynamic systems and shows how the library was adapted to these demands. As an application of TechThermo the simulation of the storage system of a solarthemal power plant is presented.

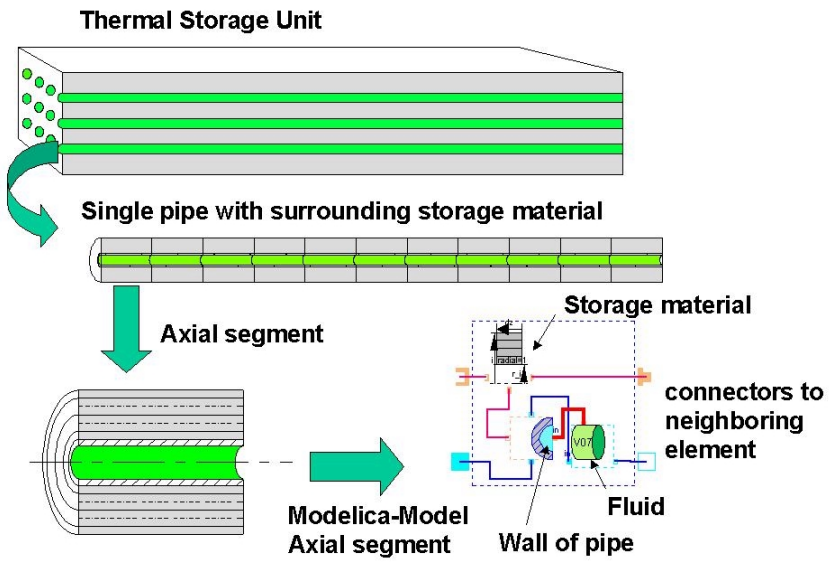

Fig.3: Modelica model for the simulation of the thermal storage system of an solarthermal power plant.

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MODELLING AND SIMULATION OF SPACECRAFT ATTITUDE DYNAMICS

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Attitude and orbit control are fundamental tasks for the operation of modern spacecraft, as both the survival of a satellite and the achievement of its mission goals usually depend strongly on the ability to maintain a desired orientation in space (or, e.g., carry out predefined attitude maneuvers) and track a desired, nominal orbit in spite of the presence of external disturbances. In addition, the recent trend towards the replacement of large, expensive spacecraft with constellations or formations of smaller, cheaper satellites, has led to the formulation of even more complex control problems, related to the relative motion (both in terms of attitude and position) of more vehicles at a time. However, spacecraft designers are also faced with a general reduction of space programmes budget, especially for scientific Low Earth Orbit (LEO) missions, embodied by the spreading of the "faster, better, cheaper" philosophy. This has resulted 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. Specific tools have to be developed for the design of both the system architecture and the Attitude and Orbit Control System (AOCS), bearing in mind the principles of reusability, flexibility and modularity. The main issue in the development of such tools should be to try and work out a unified environment to be used throughout the life cycle of the AOCS software, namely, the mission analysis stage, the preliminary and detailed design and simulation phases, the generation and testing of the on-board code, the development of the AOCS Electrical Ground Support Equipment (EGSE) and the post-launch data analysis activities. A number of commercial tools are available to support one or more of the above mentioned phases in the development of AOCS subsystems, however none of them seems capable of providing complete coverage of the whole development cycle in a sufficiently flexible way. The experience gathered in the development/use of such tools within a "signal oriented" simulation environment also showed that a more systematic approach, based on modern object-oriented modelling languages such as Modelica, might lead to the development of a spacecraft simulation library the use of which would be made much more efficient by the very nature of the selected modelling approach. Note that the use of Modelica for aerospace applications has recently led to the development of a library for flight dynamics, while, surprisingly enough, no activity in the spacecraft domain has been reported yet. Therefore, the aim of this paper is to discuss the main issues related to the modelling and simulation of satellite orbit and attitude dynamics, and to present the results obtained so far in developing a spacecraft simulation library based on the Modelica language.

MODELLING AND SIMULATION OF A MACHINING CENTER WITH DYMOLA

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Abstract. The market demand for ever increasing precision of mechatronis systems calls nowadays for a synergic design, where the mutual interactions of choices made in the mechanical design and in the drive electronics design are thoroughly understood. Dynamic performance of the machine has become the real issue, rather than static dimensioning, and dynamic performance cannot be improved unless the machine is studied with electronics and control operating in closed loop with the mechanics.
On the other hand, if design choices on the mechanical as well as on the electronic side can be tested before going on the physical prototype, through dynamic modelling and simulation, knowledge of the system is greatly improved, obviously as long as the simulation plant is a reliable replication of reality and the simulation tool is reasonably easy to use for people coming from different areas.
The general impression is that today several companies where competition and advances in dynamic precision of the machines are vital issues are somewhat ready to introduce these kinds of tools in the design process, but also that there is not enough consciousness on the real potentialities of the new approaches. Uncertainties often arise also on the requirements for the modelling language and software tool to be adopted.
This paper describes an experience of use of one of these tools: DYMOLA with Modelica language, in the simulation of a machining center.

MODELLING OF DISTRIBUTED THERMO-HYDRAULIC PROCESSES USING MODELICA

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Dynamic simulation of thermo-hydraulic processes plays an important role in the design of power plant control systems. Research has been active in this field for more than 30 years, and numerous software packages have been developed. In recent years, object-oriented modelling methodologies have emerged, in particular with the definition of the Modelica language [1]-[2]. Several application of Modelica to the field of thermo-hydraulic systems are reported [3], as well as a first attempt at developing a basic model library [4]. However, the field is still very far from being mature.
The paper discusses desirable features of a modelling and simulation environment for thermo-hydraulic processes: modularity; flexible level of detail; support of partial differential equations; open, extensible and transparent model library; substance property calculation; CACSD support; real-time functionality.
The object-oriented approach of Modelica is then compared with the equation-oriented approach of gPROMS [5] and with specialised simulation software.
Subsequently, issues arising when defining a component library for thermo-hydraulic processes are discussed, in particular the difficulties in providing basic yet general models, in defining consistent component interfaces, and in the proper use of the inheritance mechanism.
Guidelines for developing a Modelica-based modelling and simulation environment for thermo-hydraulic processes are then summarised, according to the previous discussion.
Finally, the application to the modelling of a simple process (Fig. 1) is presented to exemplify some of the general concepts presented above.

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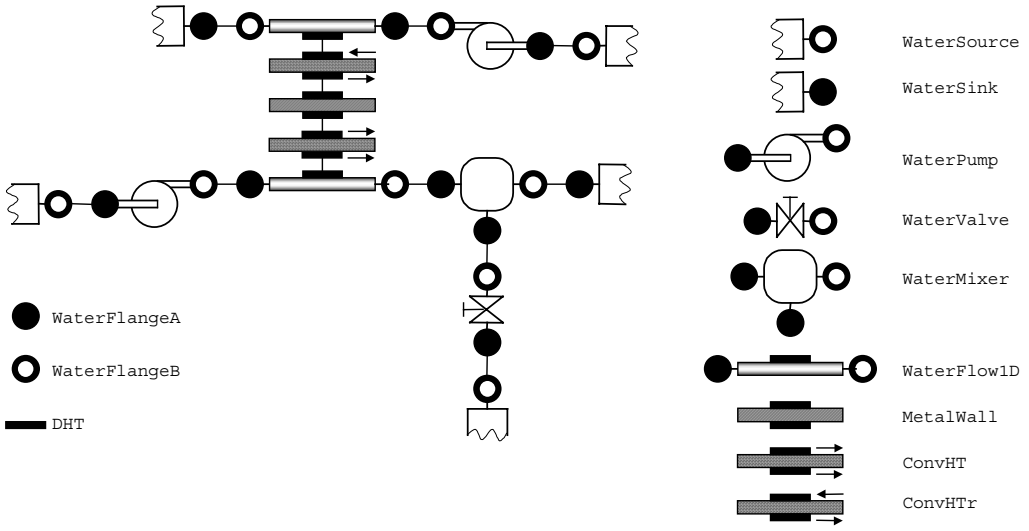

Figure 1: Object-oriented model of a simple thermo-hydraulic process.

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Fluidic Systems

POPULATION BALANCE MODEL FOR HEAT TRANSFER IN FLUID-SOLID SYSTEMS

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In modelling heat transfer in fluid-solid processing systems, three inter-phase thermal processes are to be considered: wall-to-bed, fluid-to-particle and particle-to-particle heat transfer. In systems with intensive motion of particles, the particle-to-particle heat transfer occurs through inter-particle collisions, but the studies of this heat transfer process are rather scarce [1-3].

The object of the paper is to present a population balance model developed for describing particle-to-particle heat transfer during collisions in a continuously operated fluid-solid processing system. It is assumed that both the fluid and particulate phases are well mixed, and the system through the wall is isolated from the environment. The temperature distribution of particles is described by the population density function n by means of which $n(T_p,t)dT_p$ expresses the number of particles in a unit volume of the system from the temperature the interval $(T_p, T_p + dT_p)$ at time t. Then the population balance model of the system consists of the following equations:
Population balance equation for particles:

$$\frac{\partial n}{\partial t}(T_p,t)+\frac{\partial (G_{T_p} n(T_p,t))}{\partial T_p}=\frac{q_p}{V}(n_{in}(T_p,t)-n(T_p,t))+$$
$$+k(-n(T_p,t)+\frac{1}{N}\int_{T_{p\min}}^{T_{p\max}}\int_0^1 n(\frac{2(T_p-S)}{z}+S,t)n(S,t)b(z)\frac{2}{z}dzdS, \quad t>0 \qquad (1)$$

where $G_{T_p}=\frac{dT_p}{dt}=\frac{\beta_{pf}a_p}{m_p C_p}(T_f(t)-T_p)$.

Heat balance equation of the fluid phase:

$$\frac{dT_f(t)}{dt}=\frac{q_f(T_{f,in}(t)-T_f(t))}{V}-\int_{T_{p\min}}^{T_{p\max}}\frac{\beta_{pf}a_p}{\rho_f C_f}(T_f(t)-T_p(t))n(T_p,t)dT_p, \quad t>0 \qquad (2)$$

together with the appropriate initial and constitutive equations.
(T - temperature, t - time, V – volume, q – volumetric flow rate, k – coefficient of the frequency of collisions, $b:[0,1]\to R_0^+$ - normalised probability density function of particle-to-particle heat transfer coefficient, β - heat transfer coefficient, C – specific heat, ρ - density, a – surface area. Indices: p – particle, f – fluid, pf – particle-fluid, in - input)

From the population balance equation, an infinite hierarchy of ordinary differential equations for the moments of the temperature distribution was derived which can be closed at any order. The simulation results, obtained by solving the set of ordinary differential equations of the moment equation model, indicate that the model developed provides a good tool for describing the temperature inhomogeneities of the population of particles in continuous fluid-solid systems. The model in the present form allows taking into account a number of parameters affecting the process.

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COMPARISION OF FOUR FINITE-VOLUME-ALGORITHMS FOR THE DYNAMIC SIMULATION OF NATURAL CIRCULATION STEAM GENERATORS

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The paper presents the results of a comparison of the four finite-volume-algorithms SIMPLE, SIMPLEC, SIMPLER and PISO. The analysis was done to explore and compare the suitability of the algorithms for the **dynamic simulation** of a natural circulation steam generator based on a tube-header-model (for the model see [1] and [2]). The suitability of the algorithms were tested by the help of the results of two calculation examples - a heat recovery steam generator with a horizontal tube bank and a two-drum steam generator with a vertical tube bank.
The fluid flow in the tubes is modelled one-dimensionally in axial direction. The collectors and distributors respectively are assumed to be points. The homogeneous equilibrium model is used for the two-phase flow of the working fluid with the two-phase pressure drop correlation according to [3]. The heat exchange between the fluid and the wall is governed by Newton's law and the heat transfer through the wall is assumed to be in radial direction only.
The driving force of the natural circulation is due to the difference of the density of the water in the unheated tubes and the water/steam mixture in the heated evaporator tube bank of the boiler. The most critical operation modes of a HRSG with natural circulation evaporators are fast warm start-ups and heavy load changes. In this cases stagnation or reverse flow can occur due to dynamic effects.
The flow stagnation or reverse flow as well as the change of the fluid from the state of water to that of a water/steam mixture, which is connected with a strong nonlinearity in the density - especially at low pressure systems -, causes difficulties for the convergence of algorithms.
The authors searched for an algorithm which has a robust convergence and great variation range for the under-relaxation coefficients. The computation time required for convergence was at the second place of interest. For the evaluation of the algorithm the following criterions are used:

- Variation width of the relaxation parameters, where the convergence of the method is ensured.
- Dependence of the calculation time from the under-relaxation factor.
- Dependence of the calculation time from the number of control volumes.

On the basis of the results and aims of the investigation the SIMPLER algorithm is the from the authors preferred method. The following points are decisive:

- The algorithm shows a very high stability - also in the case of a modification of the number of control volumes.
- The algorithm has a wide variation region for the under-relaxation factors and
- the algorithm has a small required under-relaxation for the calculations.

The high dependence of the calculation time from the number of control volumes is the only unfavourable of the SIMPLER-algorithm. The PISO algorithm shows compared to SIMPLER also a high dependency on the pressure coefficient. If the pressure factor is not close to 1, then the band with for the other under-relaxation coefficients decreases and the CPU time increases. The results of the SIMPLE algorithm indicates that the method has no high stability and the variation width of the under-relaxation factors was very small.

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NEURAL NET VERSUS CLASSICAL MODELS FOR DETECTION AND LOCALIZATION OF LEAKS IN PIPELINES

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Many of fluids transported by pipelines are in some sense dangerous. It is therefore often necessary to install leak-monitoring systems, especially due to legal regulations. This paper is concerned with a model-based approach – with the use of a mathematical model description of a pipeline in the form of a pipeline observer. In the case of a leak, the leak flow and leak position can be calculated. The difference between the measured and estimated flow at inlet and outlet $x(k) = v(0,k) - \hat{v}(0,k)$; $y(k) = v(L,k) - \hat{v}(L,k)$ will be referred to as residuals. $v(0,k)$ and $\hat{v}(0,k)$ denote the measured flow and the flow of the observer at the inlet of the pipeline, while $v(L,k)$ and $\hat{v}(L,k)$ denote the measured flow and the flow of the observer at the outlet of the pipeline respectively. The leak flow and position can be estimated by $v_{leak} = x(k) - y(k)$; $\hat{x}_{leak}(k) = \frac{-y(k)}{x(k)-y(k)} \times L_p$ where L_p denotes the length of the pipeline. Observer-based leak detection and localization schemes require a pipeline model to compute the states of a pipeline without a leak. The basic mathematical model of a pipeline is a nonlinear distributed parameter model. It describes the one-dimensional compressible fluid flow through the pipeline and is represented by a set of nonlinear partial differential equations. No general closed-form solution of this equations are known yet. Numerical approaches like the Method of Characteristics must be used instead. This method was realized in a special program PIPESIM which was used for the simulation of the nonlinear distributed parameters model. If the pipeline is operating in the vicinity of a working point, a linear model can be exploited. The transfer function of such model was obtained by the Laplace transformation of the linearized equations and corresponding initial and boundary conditions. The resulting transfer function was transcendent. Simple models of the pipeline in the form of a lumped parameter system was obtained by a Taylor series expansion of transcendent transfer functions. The resulting algorithm was less time-consuming and hence better suited for critical real time applications. With neural net models the gray box approach was used: The Neural net model was only an addendum to the nonlinear distributed parameter model. The inlet and outlet velocity corrections can be written as

$$\begin{aligned}\tilde{v}(0,k) &= f(p(0,k),\ldots,p(0,k-n),p(N,k-N),\ldots,p(N,k-N-n),v(N,k-N),\ldots,v(N,k-N-n))\\ \tilde{v}(N,k) &= f(p(0,k-N),\ldots,p(0,k-N-n),p(N,k),\ldots,p(N,k-n),v(0,k-N),\ldots,v(N,k-N-n))\end{aligned}$$

These two equations were realized by two neural nets. A three layers (3+8+1 neuron) neural net has proven itself as suitable trade-off between complexity and time needed to be taught. A tapped delay line with delays of 1 to 11 seconds was used at the input which has made the neural net dynamic. The models were tested using data obtained by a leak experiment on a real pipeline with $L_p = 9854\ m$ and diameter $D = 0.2065\ m$. The stationary fluid velocity prior to the leak occurrence was 2.45 m/s. A 5%-leak rate (0.1225 m/s corresponding to 14.77 m^3/h) was generated at $t = 473\ s$ at 56.4 % of the pipeline length where the outrunning fluid was filled into a tank lorry. Deviations of the mean values of the rate and position errors for all models in percent are depicted in the following Table.

%	PIPESIM	Linear distributed	Linear lumped	Neural Net
Rate	27.1487	3.0323	3.2328	3.8471
Position	6.3811	9.6956	9.6815	0.5350

The PIPESIM program results are biased in both, the estimation of leak rate and position. This is due to the bias in the fluid velocity sensors and due to the non-modelled dynamics. All other methods exhibit a small bias (approximately 3%) for the leak rate. This is probably due to approximate evaluation of the real leak rate, which was done manually. Linear models use the working point of a similar experiment, so the offsets in leak rate (which are actually the differences of residuals) were eliminated. However bias in the estimate of the leak position remained due to non-modelled effects. Some of these effects were incorporated in the neural net model, which has the smallest bias of the estimated position.

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Modelling and Inverse Problems

DETERMINATION OF MATERIAL PARAMETERS BASED ON FIELD COMPUTATIONS AND REGULARIZED ITERATIVE INVERSION

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In the numerical simulation of elcetro-magneto-mechanical devices, the precise knowledge of certain material parameters is essential. This talk deals with the problem of extracting these material parameters from measured data, illustrated by applications in nonlinear magnetics and in piezoelectricity. So far, quite complicated and costly experiments are done in order to obtain the desired material data. We propose an approach using simple measurements and applying more sophisticated mathematical algorithms, instead. The resulting formulation of the parameter identification problem involves the solution of PDEs, and the inverse problem is nonlinear and ill-posed in the sense of unstable dependence of a solution on the data. For its stable solution, we use fast forward solvers for the respective field problem, and apply a Newton type regularization method with an appropriate stopping criterion, using regularization by multilevel discretization in each Newton step. In this context, multigrid methods for unstable problems provide very efficient solvers especially for parameter identification problems in PDEs. Finally, numerical results are shown, and applicability to other parameter identification problems is discussed.

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MODEL REDUCTION FOR SEMICONDUCTOR INVERSE DOPANT PROFILING

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We investigate the reconstruction of semiconductor doping profiles from indirect measurements of device characteristics, such as voltage-current and voltage-capacitance maps. Our starting point is the identification problem with the well-known drift-diffusion system as the underlying model, which leads to a large-scale inverse problem that is difficult to handle theoretically as well as numerically. Under certain conditions, the drift-diffusion model (and the resulting device characteristics) can be approximated by reduced models. The aim of this talk is to show how different model reduction yield variants of well-known inverse problems, which can be solved with less numerical effort in order to obtain at least a first guess of the doping profile. In addition, the mathematical analysis of the reduced inverse problems provides valuable inside into the amount of data needed for the uniqueness of reconstructions.

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RECOVERING VOLATILITY IN THE BLACK-SCHOLES MODEL

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In a Black-Scholes world prices of financial derivatives depend, for known inerest rate and dividend yield, solely on the local volatility of the underlying. Market prices of liquidly traded options, such as Vanilla Calls, are directly observable on financial markets and can be used for estimating local volatilities and thus calibrating the model to the market.
The problem of volatility estimation is, like many parameter estimation problems for partial differential equations, in general illposed and has to be regularized. We formulate this inverse problem by means of the dual (Dupire) equation, which approach is fundamental for both, analytical and numerical considerations. The inverse problem can be regularized via Tikhonov regularization. Stability and convergence results are derived for a wide class of parameters, i.e. bounded volatilities with gradient in L_2, and various observation spaces (continuous, discrete in time, discrete in time and state).
For convergence rate considerations, we derive a closed form expression for the adjoint of the Fréchet derivative of the Tikhonov functional, which can be used for effectively calculating gradients, which are needed for any descent algorithm for minimizing the Tikhonov functional. A convergence rate result is proven for the case of time independent volatility (smile structure). The proof of the rate result suggest to use prices for digital Calls, additionally, in which case regularization can be done in a weaker norm and smoothness conditions for achieving convergence rates can be relaxed. Furthermore, the convergence rate result shows global uniqueness for the inverse problem under the given conditions.

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Shape optimization of optical waveguides

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Tapered waveguides – where the cross-section varies monotonically and continuously along the propagation direction – are widely used in photonics to couple light between waveguides of different shapes. It is well known that the power lost through the taper side-walls decreases for increasing taper lengths, becoming effectively loss-less or "adiabatic" for large lengths [1]. This is due to the fact that if the cross sectional variation is slow enough over length-scales corresponding to than intermodal beatlengths, the cross coupling between guided modes becomes negligible. For practical reasons however, it is desirable to keep the taper length as short as possible.

In this study we describe a technique we successfully used to create novel designs of very short injection devices capable of efficiently transmitting light from large input devices to small output devices. We then discuss the results we obtained for an example problem, and the possible applications.

We consider a glass uniform waveguide (refractive index 1.51) interfacing to air, with a width of 7 μm. The output waveguide is of the same material, but with a width of 0.5μm. We choose the working wavelength to be 1.51 μm. In this presentation we consider a two-dimensional model of this structure. The same design approach, however, will work for more general 3D structures.

We begin with choosing the trial initial shape to be a linear tapered profile. This means that the taper has an angle of 45 degrees. We therefore expect the losses to be very high. We note that for adiabaticity to be achieved we would require lengths greater than 40 μm, i.e. at least 6 times this length.

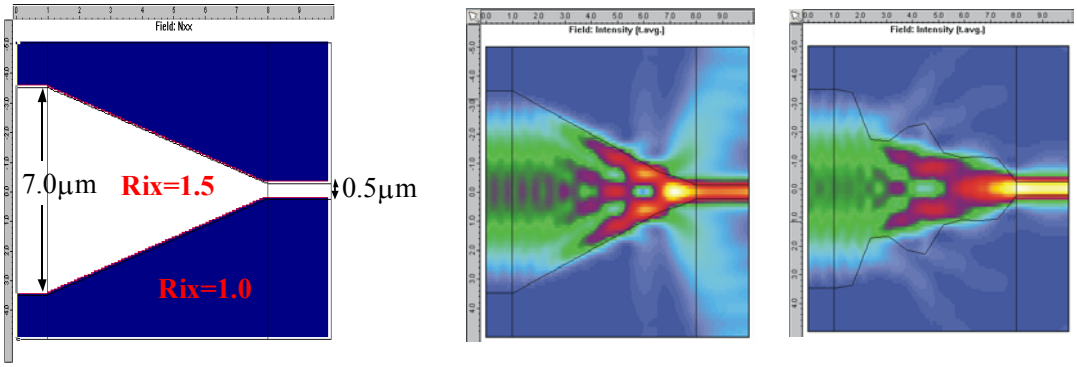

Fig. 1. Right: Initial 2D model of an injector design. Centre: The linear taper model has an efficiency of merely 53%, most of the power being lost to radiation. Right: the optimised structure with over 90% efficiency.

The aim was to improve the taper transmission by varying the taper shape, while keeping the total length fixed. Fig. 1 shows the shape we obtained after the optimization process, by restricting ourselves to the class of piecewise linear functions (fixed number of nodes). The interesting field pattern appearing in the optimised structure indicates that this highly optimal transmission is not due to an increased adiabatic effect, but to the exploitation of resonance effects between the local modes. Indeed, these interact in such a way that any power initially coupled into higher order local modes, is re-injected into the fundamental mode at the RHS exit. We then discuss how to improve on these results, and the problems encountered by increasing the discretisation of the shape. The latter can lead to instability issues due to the "inverse problem" nature of the optimisation process which appear when using high shape discretisations [2].

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Advanced Modelling and Virtual Reality Methodology in Geotechnology and Geoscience

A 4D modelling concept using NURBS applied to geoscience

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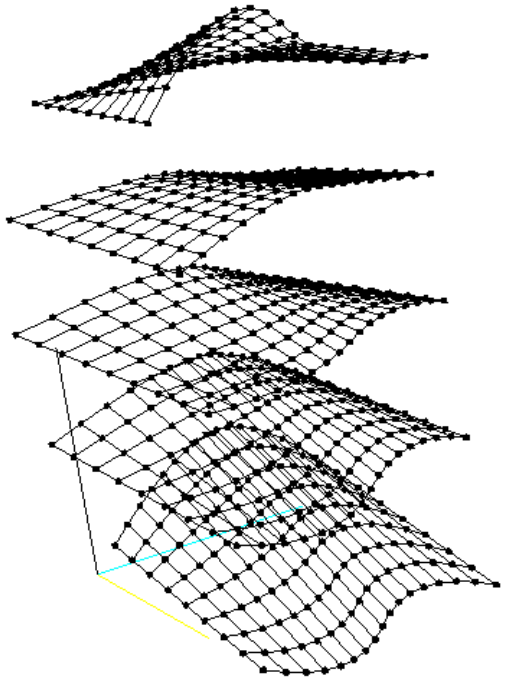
This is an introduction to the homogeneous modelling of spatial and non spatial data in 4 dimensions, i.e. space and time, utilizing 4 dimensional Non-Uniform Rational B-Splines, V(olume)T(ime)-NURBS, [1]. The proposed model benefits from its compact (vector)analytical, closed form, distinguishing it from discrete approaches like finite elements and offering properties which are especially suitable to handle a wide range of geoscientific issues:



A volumetric NURBS model represented as a set of surfaces

- Fuzzy and inexact geometries need to be represented in a realistic and efficient way.
- Missing and uncertain data should influence the model only locally.
- Handling of inhomogeneous data within a single object
- Non spatial information, like physical properties of a material within single objects needs to be represented.
- Real three-dimensional data i.e. non convex, non 2½D data representing volumetric objects must be processed, modelled and rendered.
- Heterogeneous and highly associative thematic data must be processed and *connected* to spatial information.

VT-NURBS are a potent method of modelling complex spatial and thematic processes in a similar fashion. Their compact vector-analytical form supports the accurate computation of e.g. the derivatives at a given point in a rather smooth way compared to discrete approaches. They allow the same mathematical representation for spatial and thematic information which may thus be handled in a homogenous manner (non rational case here):

$$\sum_{i_u}\sum_{i_v}\sum_{i_w}\sum_{i_t} N(u)N(v)N(w)N(t)P_{i_u,i_v,i_w,i_t}$$ with

$P_{i_u,i_v,i_w,i_t} = (x, y, z, a_1, ..., a_n)$ where the a_i represent non spatial information. These advantages can be extended to other fields like software engineering, computer graphics and non-mathematical data modelling if the VT-NURBS are embedded into the proposed object-relational data model which offers especially support for visualization and for modelling aspects which are unrelated to attributes representable as control points. This combined object-relational data model, CORE, its spatial and temporal extensions GeoCore and MoreTime are - in conjunction with VT-NURBS - imperative for the design of a data model emphasizing heterogeneous data, dynamically interconnected (associative) data, type (class) reuse, type inheritance, polymorphism and a tight bound between data and operations on this data [2].

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A time and space continuous model of salt leaching processes in a flooded potash mine

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Abstract
In 1972 the last potash mine in the Stassfurt mining district (Germany) was closed and completely flooded with brine until 1979. The flooding was followed by long-range subsidence. The brine-filled cavity volume of the entire mining district arises more than 21 million m³ until now. Since wide areas of Stassfurt city are lowered up to 4 m beneath the natural ground-water level consequently a daily drainage of approx. 1000 m³ is necessary to avoid partial flooding of the historic city of Stassfurt. These circumstances lead to a self stimulating cycle of drainage, leaching and fresh water inflow followed by subsidence. Therefore although the actual flooding is finished, underground salt leaching processes still proceed resulting in active subsidence accompanied by serious danger of sudden falling sinkholes.
In order to reconstruct the leaching process accurately, a model under consideration of the mining situation and all mechanical and hydrological parameters is indispensable. It has to unify the hydrogeochemical leaching process and its consequences for the mechanical character of the excavations with geometrical and hydrological changes in time.

Aiming a comprehensive representation of geochemical underground leaching processes in salinar rocks with associated time variant changes of cavern shapes, a temporal Geo-Information System (TGIS) is to be developed involving a data-base management system and an object-oriented process model based on Volume-NURBS (non-uniform rational B-splines) supplemented by 4D-visualisation-techniques.
Different types of salinar rocks and brine filled cavities are represented as Geo-objects (free form bodies) and treated uniformly as temporal Volume-NURBS, respecting their geochemical and physical properties. In addition to thermodynamic calculations (speciation-solubility, reaction path) underground leaching processes in salinar rocks can be specified by solution restricting processes, e.g. recrystallisation leading to partial sealing (masking) of rock surface and accumulation of insoluble substances (blocking). Within the complex system of shape changing processes uncertainties and lacking data are to be considered. Process model and data are to be managed within an information system, providing methods for time- and space-continuous representation (TGIS).

At the Institute of Geotechnical Engineering and Mine Surveying at Technical University of Clausthal the development of an adequate model is intended. A project in this regard, supported by the German Research Foundation (DFG, code number BU 1283/4-1), has started in the beginning of 2002 with a runtime of at first two years. The project, titled *Analysis, Modelling and Simulation of recent salt leaching processes in old mining cavities*, is directed by Univ.-Prof. Dr.-Ing. W. Busch. It is part of the interdisciplinary research cooperation: *Development and Application of Geoinformation to analyse Impacts and Predictions of anthropogenic influenced Processes in Geosystems*. The cooperation includes the Institute of Computer Science at the University of Hamburg, Germany, directed by Univ.-Prof. Dr.-Ing. D.P.F. Möller.

MODELLING SPATIOTEMPORAL OBJECTS AND PROCESSES AS A BASIS FOR MONITORING THE ENVIRONMENTAL INFLUENCES CAUSED BY DEEP HARD COAL MINING

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Deep hard coal mining up to 1.500 metres under ground surface often results in significant effects on elements of the anthropologic landscape and the natural environment. Existing law, especially the european directive for the environmental Impact Assessment (EIA) regulates, that projects with significant environmental effects must describe these impacts, before consent is given. Mining activities are very expensive and must have a planning reliability of 15 years and more. For intervals as long as these a forecast of the mining caused surface subsidence and combined with this the accurate estimation of environmental effects is not very reliable. This makes a short term environmental monitoring necessary and requires a verification of the consent, possibly every two years. To support the monitoring it is essential to use computer applications like geographic information systems (GIS) and database management systems (DBMS).

Even if the developments of the last few years must be called huge milestones especially to GIS, time as a further dimension is not implemented in the commercial-off-the-shelf GIS by now. Especially this is an essential in supporting monitoring tasks.

So what is time and space? To understand and describe what happens in the real world the physical space is used. The physical space in classical physics is defined by Newton. Newton distinguishes between absolute space and time on the one hand and relative space and time on the other hand. Relative space and time are movable parts of absolute space and time.

In everyday life different models of time and space are in common use. These models always hark back to the Newtonian view and can be found in every computer applications deal with space and time.

Basic approaches to integrate time in GIS were made in the last two decades, like the cartographic time, the bitemporal time, time topology and so on. Main elements of a temporal GIS are: state, event, episode and evidence. These elements can be used to describe time dependent objects.

In addition to these approaches conceptual models were defined, most of them with the main focus on the spatial object view (vector model):

- Snapshot Model: Complete area under investigation must be brought into GIS every time point.
- Amendment Vector Model: The initial state and changes at later time points are mapped. With the algebraic topology the state at every time point can be reconstructed.
- Spatio Bitemporal Model: Enhancement of the amendment vector model using valid and transaction time.
- Object-Oriented Model: object-oriented concepts are used to model the spatiotemporal system. Standards like the spatial and the temporal schema from ISO were defined, but regrettably no standard depicts the spatiotemporal characteristics of geographic information. So a conceptual object-oriented spatiotemporal model was defined integrating existing standards and existing models integrating space and time.

Fundamental aims of monitoring environmental impacts caused be deep hard coal mining, among other things are detecting changes of the earth surface or ground water surface. In general these things are modelled as time-dependent spatial field views (raster model). Some conceptual models regarding these needs could be:

- Three Dimensional GRID: with voxels a three-dimensional tessellation of two-dimensional space and one-dimensional space is possible.
- Regular Point Raster With Space-Time Paths: space is represented as a two-dimensional regula point raster. Every location has linked measures of states and / or change and also a theory of interpolation or approximation to calculate the state at every time pint on the time axis.
- Three Dimensional TIN Model: a three-dimensional triangulation can be used to interpolate elements state or change from measured parameters at known locations to different times.

The object-oriented approach can be used to model spatiotemporal objects and processes including most of the basic depicted approaches. Many of them can even be realized with data models used from today's commercial-off-the-shelf GIS and DBMS.

Virtual and Augmented Reality: An Advanced Simulation Methodology applied to Geoscience

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Virtual Reality (VR) is the methology for 3D space generation based on computer graphics and computer visualisation. VR allow user an interactive and intuitive goal-oriented interaction in real time behaviour scenarious. The potential of VR is the visualization of complex real world processes, which allow users a much more simpler handling as in reality. This result in new man-maschine communication and interaction with many new application domains behind.

Augmented Reality (AR) deals with the combination of real and virtual environment. The AR system support the user, based on semi-transparent output devices, with the computer based information needed. This means that the images, the user see on the AR device has the geometry dependent right perspectice in correlation to th real world scenario.

Our motivation for virtual and augmented reality and hence virtual and augmented environment is to go one step beyound ubiquitus computing. The basic idea of ubiquitous computing is that a single computer should not be the locus of computation in one´s research laboratory, research and design center, business or other environment. Technology should be embedded and/or distributed in the environment in an invisible as well as in a transparent way. Within this virtual and/or augmented reality environment there are tons of computationally driven gadgets or so called smart applications throughout, each could be part of a lrger system of combined devices, receiving and transmitting signals as from abroad or from intrinsic pathways. Moreover simulation within virtual and augmented reality use the power and flexibility of these methodologies with the insight of ubiquitous computing stated as computation in space and time. Due to the intuitive interaction within the virtual and augmented reality methodology normally arrousing interface problems are not the point of conflicts. This is of importance working together in transdisciplinary projects. Moreover the integration of modern 3D-control mechanisms like head mounted devices, cyber gloves, spaceball etc. enable users navigation through virtual worlds. The effect of immersion, meaning the realization of space depth, allow the user a very fast adaptation to processes in space and time. Due to that fact, new scenaric presentations are possible, containing branch specific elements and knowledge. Hence virtual and augmented reality offer a concept for modeling and simulation of complex systems with parametric as well as nonparametric topologies within a unique framework. This results in rapid prototyping, based on flexible virtual and augmeneted reality modeling tools with concepts for geometry, motion, control, as well as virtual and augmented reality components like images, textures, voice, animation, multimedia, video, etc. Applying the virtual and augmented reality methodology to the geoscience and geotechnology domain could be stated as combining distributed virtual environments, in order to support collaboration among geographically distand team members developing plans and procedures, doing measurements and dataprocessing, e.g. in a tunnel-project, in order to attempt to manage new investigations and organizational purposes, as it is needed in global as well as international project development. One of the most interesting new paradigms in virtual and augmented reality methodology in this domain is that 3D representations are not only the lonely possibility of a setting. Many virtual and augmented space applications in geosciene and geotechnology, if not already now, will in future make use of specific graphics. The virtual space can be visualized in space, which means in terms of three dimensions, and time. People in charge with virtual and augmented reality projects in geoscience and geotechnology are able to interact image based within space and time, e.g. like flighing through a tunnel, or interacting with other participants through a graphical user interface. The interweaving of functionality, distribution, efficiency, and openess aspects is very noticeable in computer graphis. The virtual space is graphically visualized flamboyance and for the most part the people in charge with the outer space application domain should see the same image. In a real geotechnology tunnel building project, irrespective of the number of participants, a state change in the virtual space needs to be communicated to all in charge with the project., using modeling and simulation techniques embedded in virtual and augmented reality.

Dynamic depth triangulation of large NURBS surfaces in real time and its application to Geoscience

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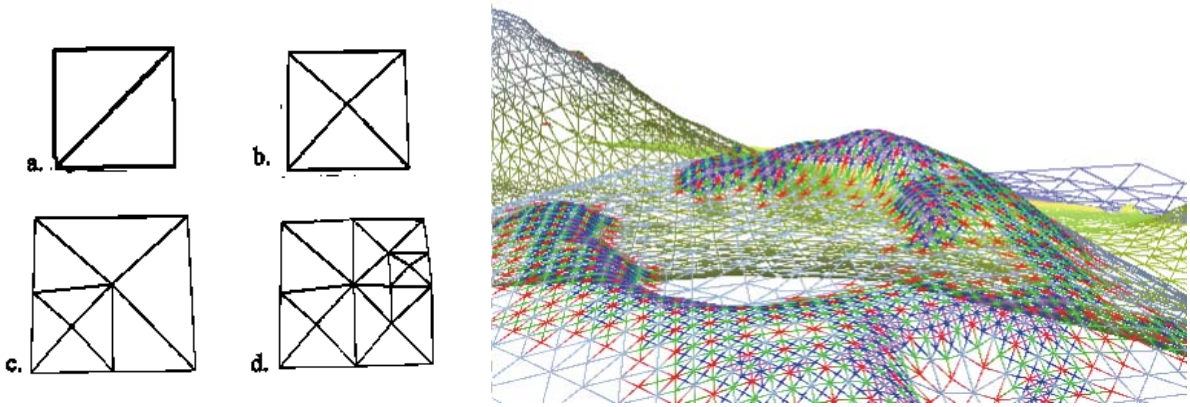
This paper presents a method on how to store and render very large NURBS-surfaces, which would be too complex otherwise to be evaluated during runtime while maintaining a proper frame rate at the same time. This can be accomplished by applying the terrain LOD technique ROAM on the NURBS' parameter plane. The result is a NURBS surface which adapts its local detail dynamically depending on the view point position and thus is especially well suited for the real time triangulation of NURBS surfaces in VR environments.

NURBS, Non Uniform Rational B-Splines, are vector valued polynomials with a number of properties making them a favored modeling tool, mainly utilized for industrial design but increasingly used as a representation for terrain. NURBS benefit from vector analytical methods and support the modeling of geological and -technical terrain properties not expressible by height fields, i.e. real 3D terrain. Standard application programming interfaces often support NURBS evaluation, but this support is usually constrained and prohibitive slow, because evaluating a point on a NURBS surface is computationally expensive. We introduce a method which applies an approach for height fields on the parameter space of the NURBS surface, allowing its triangulation in real time and supporting virtually unlimited detail.
The key to terrain rendering lies in Level of Detail (LOD) i.e. rendering those parts of the terrain which are far away from the viewer or which are rather smooth with less detail, i.e. less triangles and those parts which are close to the viewer or which are rough with more detail. [2] introduced a method for height field LOD (ROAM) which can be applied on the parameter plane of the NURBS surface and hence on the NURBS surface itself.



Dynamic NURBS triangulation : The first recursions of a triangle binary tree (left) and a highly detailed NURBS triangulation with additional detail computed at run time (right).

This approach embeds precomputed points of a NURBS surface into a recursive tree structure, which supports a different refinement at different areas and thus allows an adoption of the triangulation to the position of the view point. The algorithm could be extended by introducing a caching scheme for NURBS surface points evaluated at runtime, thus preventing the expensive re-evaluation of NURBS points at successive frames and supporting as much detail as required.

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A NEW APPROACH MODELLING IMPACTS OF MINING RELATED SUBSIDENCE ON HYDROLOGICAL PARAMETERS

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The spatial and temporal dynamics of ecological changes in mining influenced areas are driven by the amount of surface movements, local groundwater condition and the topographic situation. Additionally time–dependent changes of hydrological and ecological parameters are caused by land-use and land-cover alterations. The local intensity of the influence is determined by the relief and by local characteristics of soil and vegetation. The determination of the main components of this dynamic system forms the basis for an effective monitoring.

These analyses are a starting point to develop methods for efficient long-term monitoring procedures, taking dynamic parameters of geo-system into account. To describe dynamic hydrological and ecological processes a conceptual model has to be developed, modelling lateral and vertical water flows in consideration of different relief characteristics, soil types and vegetation covers. A pre-condition therefore is the formal description of hydro-geological structures which influence these processes. This approach has also to consider and evaluate different procedures and techniques for spatial regionalization of the model-relevant data to develop methods for a scale-independent treatment of different data layers.

The discretization of the geo-system in individual 0D to 3D-geo-objects is based on geometrical parameters, topological attributes and thematic characteristics taking the hydrological and ecological situation into account. The goal is the space and time-variant (3D/4D) modelling and visualization of the area under investigation using the information system $BAGIS_{VR}$. This system is currently under development. The core of $BAGIS_{VR}$ consists of an object-relational data base management system, as well as a new approach for the representation of time-dependent and process-oriented geo-objects by temporal 3D-Non-Uniform Rational B-Splines (TV-NURBS). The analysis and evaluation of the occurring changes for known and calculated surface movements form the basis for the derivative of functional dependencies between these geo-objects. Due to complex and ambiguous interactions between the compartments of the geo-system as well as hydrological and ecological parameters an abstraction of the model is necessary. Therefore the description of the interactions between the geo-objects takes place via statistical methods and procedures like the fuzzy set theory. The application of this model will allow simulations under consideration of additional surface movement variants.

This is part of an interdisciplinary research project *"Development and application of geoinformation to analyse impacts, predictions and management of anthropogenic influenced processes in geosystems"* – sub-project: *"Analyses of landscape-ecological changes caused by dynamic surface movements resulting from mining activities"*. The project is carried out conjointly with the Institute of Computer Science of the University of Hamburg directed by Univ.-Prof. Dr.-Ing. D.P.F. Möller and is supported by the German Research Foundation (DFG, DFG-ID: BU 1283/3).

NEURAL BASED CLASSIFIERS APPLIED TO COMPLEX GEOSYSTEMS ANALYSIS

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The employment of neuronal-based classificators as a tool for the analysis of complex interacting natural and technical systems has won a wide spectrum of applications in the last years. However the utilization in geotechnical problems remained restricted to few areas. For example in the analysis of seismic profiles, the evaluation of mineral deposits or in geo-ecologic themes qualitative statements were derived. The main problem in the application of automatic classificators, such as neural networks, to the quantitative analysis of processes in geological systems is based on the complexity of the underlying database and on the necessity of individual data processing strategies as a pre-processing step of the neural-based analysis. The inclusion of uncertain data to the improved estimation of hydrogeologic parameters was until now a domain of geostatistic methods, especially if data values are restricted in their in amount and quality. As an alternative strategy to these methods combinable neural net modules are presented for the analysis of data from hydrogeological and geomechanical investigations in the area of the Leibis/Lichte dam site in Thringen. A procedure has been developed and evaluated, that allows the analysis of multivariate systems on the basis of artificial neural networks with a linked high end visualisation technique.
For evaluation the relevant data out of different phases of the dam project were assembled and structured in a relational datamanagement system. The developed program modules contain query structures that permit a problemoriented access on the total database. Methods that allow to create any provided possible combination of feature-vectors as input patterns of the neural net are given. The single features of these vectors are preprocessed by procedures of fractioning and/or standardization strategies. So freely combinable test and training data sets can be developed, and can be presented to different independent network topologies. The result values of the neural classification process are visualised three-dimensionally as different hydrologic and geomechanic main values. Possible results are represented as a probability value of flow velocities, flow directions, grouting effectivity of the rock mass in dependence of the location and the shaping behavior of different fracture generations in a spatial model, based on an advanced neural computing method, that could be described as a multi-dimensional selforganising feature map.
As a new visualisation technique, the concept of Volume Non Uniform Rational B-Splines, (VNURBS) was combined with the neural network classification module. In combination with modern database management systems, this will lead to specific information systems for geotechnical applications, that will help to cope with the high information flow in complex projects.

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Modelling and Decision Support for Environmental Systems

A GENERAL CONCEPT OF ECOSYSTEMS USING CATEGORY THEORY

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Within the various interpretations of ecology different concepts of systems theory play a central role. Ecosystems are open systems for energy and matter characterised by non-equilibrium processes and multiple stationary states (Gnauck and Straskraba 1980). They can be understood as control systems with stochastic disturbances. A general system description used in state space theory, dynamical system theory and automata theory is given by nonlinear and instationary multiple operators F and G where $F: X \times U \rightarrow X$ with $x = F(x, u)$ and $G: X \times U \rightarrow Y$ with $y = G(x, u)$. The operator F transforms the changes of inputs into changes of states, and G transforms the changes of states into output changes under consideration of internal and external disturbances. In this cases ecosystem models are presented by differential equations describing the changes of systems behaviour in space or time. Another way to model ecosystems is the use of automata theory (Arbib 1968) and the theory of categories as parts of the algebraic theory (Benabou, 1963; Budach and Hoehnke, 1975) where morphisms between the ecosystem components are represented by stochastic functions (Rosen 1971). Each ecosystem and also its subsystems or components will be understood as a stochastic automata (S-automata) whose changes of states are decsribed by discrete measures of probability. The interpretation of an abstract automaton A as an algebraic structure S leads to an algebraic automata description and consequently to formulations by category theory. One goal of application of algebraic methods consists of an unified and general mathematical description of the biocoenotic structure and functioning including stochastic interrelationsships within the system and with its environment. Therefore categories with multiplication are used to explain theoretically the ecosystem behaviour. An ecosystem is represented by a category *C-Mat* which result from *C-Aut* categories by an inclusion functor *Inc(C)*: *C-Aut* $\rightarrow$ *C-Mat*. In *C-Mat* exist special morphisms: Exchange morphism, diagonal morphism, terminal morphism, canonical projection (product). The imbedding of sub-categories into the the category *C-Mat* will be realised by an imbedding functor *Imb(C)*. On this way it is possible to describe trophic levels or single elements of an ecosystem as sub-categories which are imbedded into other categories. Single elements will be called elementary automata, their morphisms represent elementary switching circuits. In the sense of information theory, stochastic automata are transmission channels with information being taken in, stored, processed within the system and transmitted back to the environment. The S-automata operate on a certain scale with enumerable infinite strokes. For each stroke the S-automata gets a set of input signals, releases a set of output signals and has exactly one set of well-defined states. Combining switching operations of elementary automata with internal and external couplings the behaviour of an ecosystem may be described algebraically where parallel and serial couplings and combinations with other automata operations are included. The result of this approach gives an unifying concept reflecting the stochasticity of structure and functioning of an ecosystem.

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VALIDATION OF A SHALLOW LAKE MODEL

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The subject of this contribution is the eutrophication model HavelMod which is applied on the river stretches and shallow lakes of the Havel. Its' basic concept which is shown in Fig. 1 has been developed in consideration of Lijklemas' recommendation (1993) only to include the essential processes. In the case of the waters mentioned above the interaction between the sediment and the water column can be seen as "essential" for the processes of early diagenesis have a great influence on the balance of algae and nutrients. As a whole the resulting mathematical model is a simple system of six ordinary differential equations including one equation for the diffusive flux of phosphorus between pore water and water column.

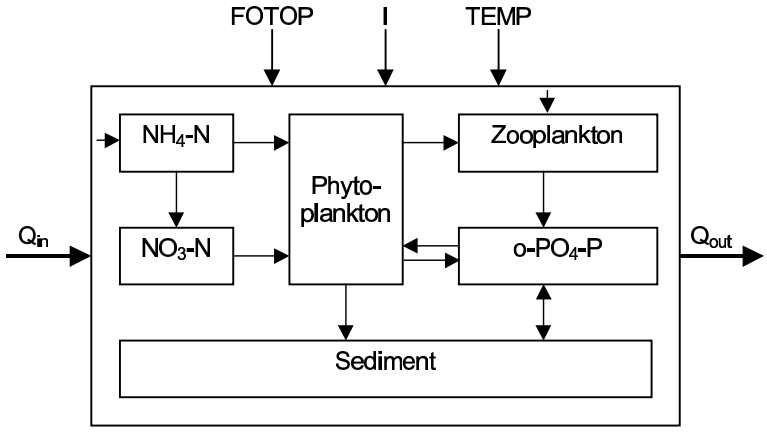

Fig. 1. Model concept of the eutrophication model HavelMod.

The demand after simplicity can be traced to the goal of an efficient calibration and use of the model. A high grade of particularization may deliver a good concept model but when its corresponding numerical model cannot be handled suitably the modeler will probably fail in the validation phase. HavelMod can be taken as an extensible basis which may be developed further by the support of mathematical optimization algorithms.

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MULTICRITERIA DECISION SUPPORT FOR WATER QUALITY MANAGEMENT OF RIVER BASINS

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Simulation models for water quality management (WQM) including optimisation mainly deal with some form of cost minimisation designed to meet environmental quality and/or ecological standards. Pollution regulations are specified either in terms of river water quality or in terms of effluent standards. Most often the goal is a suitable control scheme which present a compromise between the available budget for prevention measures and an acceptable water quality (Cembrowicz 1988). In this context, river basin management (RBM) strategies have to consider economical and environmental objectives. They require decisions which are based on multiple contradictory goals, on different evaluation procedures and on distinguished valuation scales (Steuer 1986). Most of the RBM problems arise due to interactions between throughflow, discharged soluble and suspended matter, natural and man-made chemical substances and environmental influences from the catchment. Therefore, extended DO-BOD models and eutrophication models have become widespread in RBM studies (Wierzbicki et al. 2000). Such models must be capable of depicting the hydrological, chemical, and biological processes occurring in the river adequately, while incorporating economical and ecological considerations within the decision framework. This implies that a multi-goal environmental process will always be understood as a search for acceptable compromise solutions. Pareto-optimisation seems to be such a method to evaluate multi-goal functions. Then, decisions are based on scenarios resulting from optimised outputs of simulation models. The paper gives an short overview on model based decision support systems (DSS) for RBM. The special DSS REHSPROX was used to compute Pareto optimal solutions of the DO balance of the rivers Spree and Lower Oder. The following types of data were used for simulation and optimisation:

1. *River water quality data*: DO, BOD, water temperature;
2. *Data of WWTPs*: effluent DO, effluent BOD, discharge of wastewater;
3. *River morphometry and hydrology*: average depth, average width, average volume of river segments, average flow velocity within each river segment.

The goal functionals for the DSS REHSPROX are formulated by the following expressions valid for all segments and all time steps: $\max\sum^{i}\sum^{t}DO(t)$, $\min\sum^{i}\sum^{t}BOD(t)$, $\max\sum^{i}\sum^{t}QE(t)$ and $\min\sum^{i}\sum^{t}IC(t)$. To get an information on the domain of decision the individual optima of the variables under consideration are computed. In the paper, results of Pareto optimisation for the Rivers Lower Oder and Spree are presented. According to these results optimal cost functions for investments are presented.

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THE ECOSCAPE FRAMEWORK FOR SPATIALLY EXPLICIT MULTIPLE-SCALE MODELLING OF ENVIRONMENTAL SYSTEMS

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Hierarchical, asymmetric cellular automata (HACA) have been introduced in [Sonnenschein and Vogel, 2001/2002] for spatially explicit modelling of ecological systems and land-use modelling. The modelling method is primarily motivated by the well-known scale problem of ecological systems [Levin 1992]: process dynamics of such systems can be observed on different spatial and temporal scales influencing each other. HACA overcome the restrictions of traditional cellular automata for modelling such multiple-scale systems by introducing the following concepts:

- Cells of different spatial scales are hierarchically organized by aggregation into levels.
- Each level of cells has its own time scale for state changes in this level.
- State changes of cells in one level may depend not only on the cells in this level but also on the state of corresponding cells in the neighboring levels.
- The structure and the dynamics in one level of cells are based on asymmetric shaped cells, irregular neighborhood relations, and external influences to cells.

We introduce an object-oriented programming framework EcoSCAPE written in C++ which supports the creation of any model based on the formal framework of HACA. This programming framework facilitates the creation and simulation of models by means of object-oriented concepts, e.g. inheritance. Although a scripting language for defining rules and neighborhood relations is not yet realized, EcoSCAPE is designed to create models during applications runtime. This run-time modelling feature will allow the implementation of a general and interactive graphical modelling tool which exempts the modeler from programming tasks.
The EcoSCAPE framework supports the persistency of models by using an XML data format for storing them. The different aspects of a model at run-time, i.e. its structure, scenario and state, can be saved and loaded separately. EcoSCAPE provides a general persistence interface which is not forced to a definite storage format. So it is easily possible to define other data formats for models.
EcoSCAPE supports the integration of data stored in external databases: Geometrical data may be used for the definition of a cell's shape whereas thematic data may initialize the cell's state values. This provides an easy use of 'real world' objects. A concrete database interface to the geographical information system InterGIS® demonstrates the use of the frameworks abstract database interface.
The framework has been successfully used on the operating systems Linux and Microsoft Windows® and is documented by an API reference, a tutorial, and the application example 'EcoLIFE'.

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Geoinformation Systems and Environmental Systems

ABSTRACT
COUPLING OF GEOGRAPHIC INFORMATION SYSTEM AND SYSTEM DYNAMIC MODELS
(A regional spatio-temporal soil erosion model implemented with ArcMap and Vensim)

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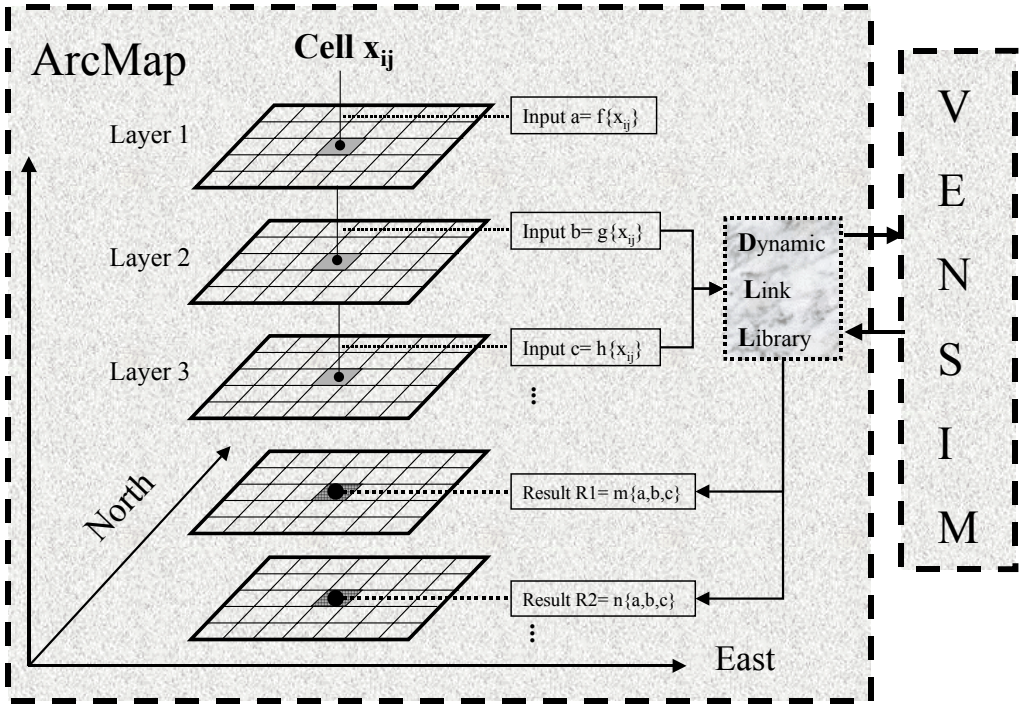
During the last few years a continuously increasing amount of geographic information has become available. This data could be very valuable for environmental models. Geographic Information System (GIS) software offers only limited possibilities to build models compared to special dynamic modelling software. The aim of the study was to make use of available spatially explicit data within a dynamical modelling software. Data processed by ArcMap, a GIS-Software, were transferred into a suitable format, to serve as input for a model built in Vensim, a system dynamic modelling software. Finally, the results from the simulation were returned back to ArcMap for further processing and visualisation. This procedure enables modellers to combine the advantages of both tools – to simulate the development of a given geographic region both in space and time. The developed method was evaluated for the simulation of soil erosion in an Upper Austrian catchment.
Keywords: GIS modelling, System Dynamic, Soil Erosion model, Vensim,



A tight coupling method between ArcMap and Vensim, shown in the Figure above, combines the benefits of both tools. The connection was achieved with a VBA program code and DLL functions for the communication from ArcMap to Vensim. The developed method allows not only to use both tools together, but also to use the GIS for analysing the data and the system dynamic model built in Vensim for analysing the system behaviour independently. This enables a continuous improvement of the model structure without the need to adapt both tools. The developed method provides a big step to the development of decision support systems (DSS). For environmental modelling the analysis of systems structure with causal loop and stock and flow diagrams in relation to the spatial dimension will help to refine simulation of future development – for example in the context of the Kyoto targets. Efficiency of applied environmental protection measures can be increased by targeting applications to those areas, where measures are actually needed.

AIR QUALITY ESTIMATES AND CONTROL OF INDUSTRIAL EMISSIONS

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The release of toxic gases from industrial plants constitutes a serious hazard to human health and environment. The control of industrial emissions is the problem of great practical importance and considerable mathematical interest [1,2]. During thermic inversions, the atmospheric stability is strong, the pollutants are accumulated within a thin surface layer, where the vertical structure of the process can be ignored to the first approximation. Assume that in a 2-dim urban area D there are N industrial plants located at points $r_i = (x_i, y_i)$ with emission rates $Q_i(t)$ ($i = 1,2,...,N$). We consider in D and time interval $(0,T)$ a vertically integrated (over the surface layer) model based on the advection-diffusion-reaction equation

$$\frac{\partial}{\partial t}\phi + \boldsymbol{U}\cdot\nabla\phi + \sigma\phi - \nabla\cdot\mu\nabla\phi = \sum_{i=1}^{N} Q_i(t)\delta(r - r_i) \qquad (1)$$

Here $\phi(r,t)$ is the pollution concentration at point $r = (x, y)$ and time t, $\delta(r - r_i)$ is the Dirac function of the i th plant position, $\mu(r,t) > 0$ is the turbulent diffusion coefficient, and $\sigma(r,t) > 0$ characterizes the decay of $\phi(r,t)$ due to physical and chemical processes [1]. The wind velocity $\boldsymbol{U}(r,t)$ is known and non-divergent in D. The model (1) has unique solution continuously depending on the initial distribution $\phi^0(r)$ and the number N, emission rates $Q_i(t)$ and positions r_i of the industries [1].

Let Ω be an ecologically sensitive zone in the domain D. Solutions $\phi(r,t)$ and $g(r,t)$ to the model (1) and its adjoint are used to derive two equivalent (direct and adjoint) estimates of the average pollution concentration in Ω and time interval $(T - \tau, T)$ of length τ [1,2]:

$$J(\phi) = \frac{1}{\tau|\Omega|}\int_{T-\tau}^{T}\int_{\Omega}\phi(r,t)\,dr\,dt\,, \qquad J(\phi) = \sum_{i=1}^{N}\int_{0}^{T} g(r_i,t)Q_i(t)\,dt + \int_{D} g(r,0)\phi^0(r)\,dr \qquad (2)$$

The estimates (2) are used to monitor the air quality in ecologically important zones inside D. The first (direct) estimate (2) requires solving the pollution transport problem again whenever emission rates and/or initial pollution distribution are changed. Unlike this, the adjoint model solution is independent of these characteristics and serves in (2) as the weight functions, providing valuable information on the contribution of each source in polluting a zone. It makes the second (adjoint) estimate (2) economical and convenient for the sensitivity study of $J(\phi)$ to variations in the emission rates $Q_i(t)$ and initial pollution distribution $\phi^0(r)$.

Assume that the model forecast is unfavorable in the sense that pollution concentration $J(\phi)$ exceeds the sanitary norm J_0 in Ω: $J(\phi) > J_0$. Then one of the control strategies should be applied to reduce emission rates and prevent excessive polluting the zone Ω. Three strategies that differ by the ways of restricting the emission rates are suggested. The first (optimal) strategy imposes restrictions on the total amount of the pollutant emitted by each industry throughout time interval $(0,T)$. The second (non-optimal) strategy prescribes a temporal behavior of the emission rates in $(0,T)$, whilst the third (optimal) strategy sets the greatest possible emission rates in $(0,T)$, and hence, is less restrictive and more attractive for the industries. Each strategy uses solutions to the adjoint problem and assures the fulfillment of the air quality norm in the zone:

$$J(\phi) \le J_0 \qquad (3)$$

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Mathematical modelling and simulation of river water quality

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With the background of increasing technical and legal requirements, it is important for engineers to be able to assess quantitatively and qualitatively impacts of urban drainage discharge on rivers. Prevention of water pollution increasingly becomes the focus of interest. Assessing impacts on rivers requires a detailed knowledge about river systems. Apart from measurements, engineers use typical river assessment concepts in order to explain rivers or river-sections on the basis of few easy collectable environmental parameters by separating them into regions with unique characteristics. A number of such river concepts are available. All of them refer to special economical and ecological questions such as fishing, water extraction, water protection and water quality.

In addition to experience and river concepts, river water quality models can support the work of engineers. Quality modelling means modelling biological and chemical processes and can look back on a long tradition regarding rivers. The essential impetus for quality modelling was triggered by fish-dying, caused by oxygen-reducing substances. The first steps were made in the early years of the twentieth century, with the aim to be able to predict the temporal and spatial changes of the oxygen concentration.
Various river quality model approaches have been developed in order to predict wastewater discharges. Particularly QUAL2 enjoys large popularity and was integrated into various simulation systems and adapted to special needs. The different models and programs refer to a comprehensive experience with river quality simulations, but there are some points which put the general performance capability in question.

Beside the river water quality models, models for the wastewater treatment were developed in order to predict the purification capacity. The simulation of wastewater treatment plants is meanwhile an acknowledged method supporting the design and optimisation. For a long time, both model types were separately used. Nowadays, the wastewater treatment and receiving waters will be seen more and more as compartments of one system with close connections. Integral examination of the wastewater treatment and receiving waters by using quality models is one of the interesting research topics in environmental engineering. An integrated modelling and simulation of wastewater treatment plants and receiving waters can improve the information value of investigations based on quality models. Some international research-projects for integrated modelling use a submodel of the River Water Quality Model No.1 (RWQM1) by the International Water Association. Most of them are still in preparation. Practical experience reports are hardly available. As a framework, the model has to be adapted to the special needs of an application. Because of the heterogeneity of rivers and generally little information about a river, a submodel adaptation is an interesting challenge.

The paper presents an example application, using the RWQM1, which should serve for collecting experiences with river water quality modelling in order to find out the requests, capabilities, possibilities and arising difficulties. The paper starts with a short introduction to show where quality models can positioned for the practical work. Based on the information about a real brook, the focus is put on the presentation of the main steps to set up a model. Following, some simulation results will be presented. The paper closes with an assessment of the achieved results and it tries to look out for the future direction of river water quality modelling.

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STOCHASTIC WIND MODELING BASED ON EXPERIMENTAL DATA

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To assess and predict the effect of atmospheric wind on the dynamic response and statistical characteristics of aerospace launch vehicle or aircraft, we need a stochastic model of wind filed. Such a model should recreate numerically wind as a random function of altitude. For example in Monte-Carlo flight simulation, the simulator of wind should regenerate stochastic functions, which satisfy random characteristics of atmospheric turbulence. Mathematical modeling and simulation of wind as a stochastic function fined many applications in aerospace and the others area in science and engineering [1][2].
In this work developed a simplified alternative to canonical expansion method. Canonical expansion of wind as a two dimensional stochastic vector-function may be considered as:

$$v(h) = m_v(h) + \sum_{i=1}^{k} b_i j_{vi}(h)$$
$$az(h) = m_{az}(h) + \sum_{i=1}^{k} b_i j_{azi}(h) \qquad (1)$$

Where: $v(h), az(h)$ Random functions of altitude for wind velocity and wind azimuth,

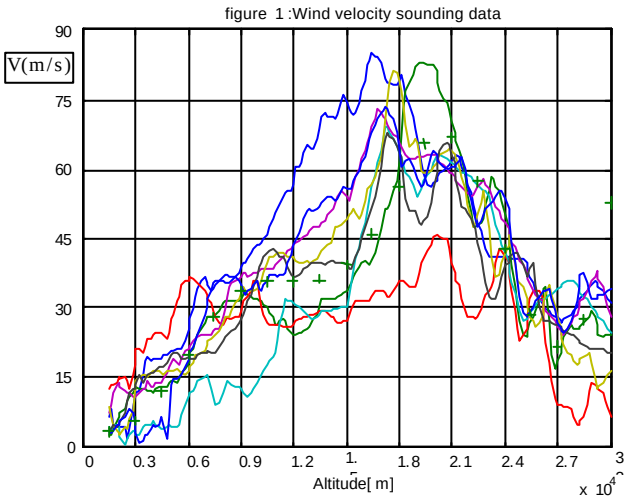
$m_v(h), m_{az}(h)$ Mean value of wind velocity and azimuth as a function of altitude,

j_{vi}, j_{azi} -Coordinate (deterministic) functions for wind velocity and azimuth,

The main problem in stochastic process modeling by the canonical expansion approach concerned with coordinate function determination [1]. This step requires heavy preliminary experimental data analyzing. In order to find a simple algorithm for wind modeling and simulation, in this paper proposed a method based on combination of canonical expansion approach and concept of random vector. In the general case, when $K_{ij} \neq 0$, the correlated Gaussian vector $\vec{X}$ can be simulated by linear transformation of the normalized Gaussian vector $\vec{b}$, consisting of the non-correlated normalized Gaussian variables $b_i (D_{b_i} = 1; i = 1,....n)$.

$$\vec{X} = \vec{m}_X + A\vec{b} \qquad (2)$$
$$AA^T = K_X \qquad (3)$$

This method eliminates complexity of coordinate function determination. Example of experimental data and simulation by proposed model demonstrated in fig 1. (By sign + indicated example of wind velocity generation)



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MATHEMATICAL MODELING OF RECURRING RADIOACTIVE CONTAMINATION DURING FOREST FIRES

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The paper suggested in the context of the general mathematical model of forest fires gives a new mathematical setting and method of numerical solution of a problem of a radioactive spread above the forest region. Numerical solutions of problems of a radioactive smoke spread during surface and crown fires in exemplified heat energy release in the forest fire front were found. Heat energy release in the forest fire front was found to cause further radioactive particles spread by the action of wind. Concentration of particles in the general crown forest fire was found to be 3-5 times greater than in the surface forest fire. In the absence of wind, radioactive smoke particles deposit again on the underlying surface after a time. As a wind velocity increases, these particles are transferred in the ground layer over distances proportional to a wind velocity. It is common knowledge that in the case of radionuclide ejection over the forest region, radionulides concentrate mainly on the soil cover (70%) later on as a consequence of their settling under gravity, and only 3 - 4 % of them settle in the tree crowns. Powerful up-currents of gas occur in surface and crown forest fires, causing entrapment of radioactive particles together with heated gaseous combustion products of forest fuels in the ground layer. Therefore radioactive forest fires cause a radioactive smoke, which spreads by the action of wind in the ground layer in the forest fire region in a wind direction. In this paper the theoretical investigation of the problem of forest fire spreading through the radioactive forest in windy was carried out. The research was made by means of the mathematical modeling methods of physical processes. It was based on numerical solution of Reynolds equations for the description of turbulent flow taking into account for diffusion equations chemical components and equations of energy conservation for gaseous and condensed phases. The method makes it possible to evaluate an overall contamination situation in radionuclide contaminated areas. In this context, a study mathematical modeling of the conditions of forest fire spreading that would make it possible to obtain a detailed picture of the change in the velocity, temperature and component concentration fields with time, and determine as well as the limiting conditions of radioactive propagation of forest, is of interest. The surface fire source is modeled as a plane layer of burning forest fuels with known temperature and increasing area of burning. It is assumed that the forest during a forest fire can be modeled as a two-temperature multiphase non-deformable porous reactive medium. Let there be a so-called "ventilated" forest massif, in which the volume of fractions of condensed forest fuel phases, consisting of dry organic matter, water in liquid state, solid pyrolysis products, and ash, can be neglected compared to the volume fraction of gas phase (components of air and gaseous pyrolysis products).

The boundary-value problem was solved numerically using the method of splitting according to physical processes. In the first stage, the hydrodynamic pattern of flow and distribution of scalar functions was calculated. The system of ordinary differential equations of chemical kinetics obtained as a result of splitting was then integrated. A discrete analog was obtained by means of the control volume method using the SIMPLE algorithm. The accuracy of the program was checked by the method of inserted analytical solutions. Analytical expressions for the unknown functions were substituted in system of differential equations and the closure of the equations were calculated. This was then treated as the source in each equation. Next, with the aid of the algorithm described above, the values of the functions used were inferred with an accuracy of not less than 1%. The effect of the dimensions of the control volumes on the solution was studied by diminishing them. The time interval was selected automatically.

Fields of temperature, velocity, component mass fractions, volume fractions of phases and concentration of additional radioactive pollution were obtained numerically. The wind field in the forest canopy interacts with the gas-jet obstacle that forms from the surface forest fire source and from the ignited forest canopy base. A great deal of final and intermediate gaseous and dispersed combustion products of forest fuels is known to be exhausted into the atmosphere during forest fires. As wind velocity increases radioactive smoke particles are transferred in the ground layer distances proportional to a wind velocity. The knowledge of these kinds of information enables a full estimate of the damage from forest fires to be made.

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Electrical, Electronic and Power Systems

AN ALGORITHM FOR SMOOTHING THREE-DIMENSIONAL MONTE CARLO ION IMPLANTATION SIMULATION RESULTS

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An algorithm for smoothing results of three-dimensional Monte Carlo ion implantation simulations is presented. This algorithm is indispensable for joining various process simulation steps, where data has to be smoothed and translated to unstructured three-dimensional grids. Its foundation are a generalization of Bernstein polynomials to multi-dimensional cuboid domains, whose properties are proven.
The usual approach is to perform a least squares fit of multivariate polynomials of fixed, low degree, usually two, and to hope to obtain a suitable approximation and that suitable smoothing takes place. This RSM (response surface methodology) approach is used extensively in TCAD applications. The new approach using generalized Bernstein polynomials was put on a sound basis and does not suffer from the adverse effects of the popular RSM.

Properties of a Generalization of the Bernstein Polynomials: After defining the generalization of the Bernstein polynomials to multidimensional intervals, we prove their most important properties like the following:

- **Uniform Convergence:** Let $f : [0,1]^m \to \mathbb{R}$ be a continuous function. Then the multivariate Bernstein polynomials $B_{f,n_1,\ldots,n_m}$ converge uniformly to f for $n_1,\ldots,n_m \to \infty$.
- If $f : I := [0,1]^m \to \mathbb{R}$ is a continuous function satisfying the Lipschitz condition $\|f(x)-f(y)\|_2 < L\|x-y\|_2$ on I, then the inequality $\|B_{f,n_1,\ldots,n_m}(x)-f(x)\|_2 < \frac{L}{2}\left(\sum_{j=1}^m 1/n_j\right)^{1/2}$ holds.
- **Asymptotic Formula:** Let $I := [0,1]^m$, let $f : I \to \mathbb{R}$ be a C^2 function, and let $x \in I$, then

$$\lim_{n\to\infty} n(B_{f,n,\ldots,n}(x)-f(x)) = \sum_{j=1}^m \frac{x_j(1-x_j)}{2}\frac{\partial^2 f(x)}{\partial x_j^2} \le \frac{1}{8}\sum_{j=1}^m \frac{\partial^2 f(x)}{\partial x_j^2}.$$

The Algorithm and a Three-Dimensional Example: The algorithm works by constructing approximating generalized Bernstein polynomials in the neighborhood of the points of the unstructured, new grid.
The new algorithm and its RSM counterpart are compared in a real world example, namely the simulation of the implantation of Boron into a a three-dimensional CMOS structure. A Boron dose of $10^{13}\,\mathrm{cm}^{-2}$ with an energy of 15 keV was implanted in the Monte Carlo simulation using an isotropic homogeneous grid. The resulting concentration of Boron interstitials in $[\mathrm{cm}^{-3}]$ after smoothing by the new algorithm is shown in Figure 1, together with the unstructured destination grid with 78 651 points. The smoothing algorithm was found to yield superior results which can immediately serve as input to subsequent simulations.

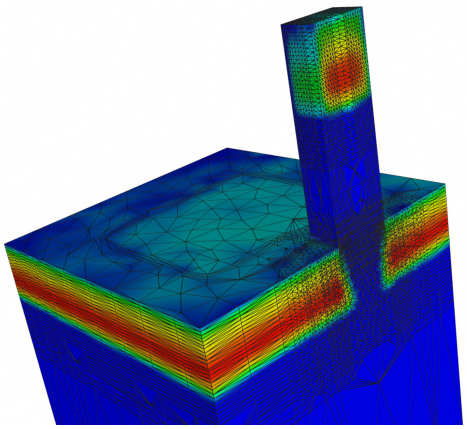

Figure 1: A front view of the sample Monte Carlo ion implantation after smoothing using the new algorithm.

DETERMINATION OF TURNING POINTS IN ELECTROMECHANICAL SYSTEMS

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The modelling of electromechanical systems as e. g. MEMS has to take into consideration nonlinear behavior. An inherent instability situation in electrostatic actuators, known as pull-in, results from these nonlinearities. The pull-in instability is the principle phenomena that limits the design of nearly every electrostatically actuated MEMS device. For instance, when a voltage drives an electrostatic parallel plate actuator, the pull-in instability limits the range of displacement to 1 / 3 of the gap. For higher voltages the plates come together. On the other hand the pull-off voltage is smaller than the pull-in voltage and depends on the remaining gap between the plates after pull-in, cf. [1]. This phenomena is also known for electrostatic actuators that are more complicated. Electrostatic actuators are used in a wide area of applications, including optical routers, radio-frequency microswitches, voltage-controlled capacitors, pressure sensors, and others. The pull-in effect may be either disturbing or useful, depending on the application. The analytical and numerical determination of pull-in points and their classification is discussed in the full paper.

Mathematically this instability can be explained by a single fold in the static characteristic of the devices under investigation. Roughly spoken, we use the following approach: A nonlinear system of equations describes the equilibrium between electrical and mechanical forces. Unknowns of this system are the applied voltage (or charge) and displacements of mechanical points in the case of a translational system. The solution of the system of equations describes a one dimensional curve in a higher dimensional space

$$\mathcal{L} = \Big\{ z(t) = \big(x(t), y(t)\big) \colon\ F\big(x(t), y(t)\big) = 0,\ t \in [t_{\min}, t_{\max}] \Big\} \quad \text{with} \quad F \colon\ \mathbb{R}^n \times \mathbb{R} \mapsto \mathbb{R}^n.$$

It contains simple singular points [2]. In particular, turning points which are the weakest singular points occur and of special interest. In fact, pull-in parameters are characterized by simple turning points. For $n = 1$ simple turning points can be easy computed by simultaneous solving of the two equations

$$F(x, y) = 0\ , \quad \partial_x F(x, y) = 0\,. \tag{1}$$

Moreover, double turning points and simple bifurcation points may arise at $\mathcal{L}$ in dependence of model $F(x, y) = 0$. In particular cases, system (1) can be analytically solved by means of Computer Algebra Systems. In general, the values of the pull-in parameters have be calculated numerically.

The evaluation of these equations leads to numerous expressions describing the pull-in parameters with respect to nonidealities of parallel plate actuators, the influence of series and parallel capacitances, torsion actuators, ... On the other hand a solution curve can be computed by a discrete set of solution points using curve tracking methods. For this purpose, the basic equation has usually be extended by a further equation. It can be shown that the original equation and its augmentation define together a network analysis problem which can be solved using state of the art network simulation programs that can include user elements described by standard hardware description languages like VHDL-AMS [3]. At a simple turning point an event on the implicit signal `y'DOT'ABOVE(0.0)` occurs.

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ANALYSIS OF POWER SYSTEM DYNAMICS IN CONSIDERATION OF LOAD CHARACTERISTICS WITH CONTINUATION METHODS

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Electrical power systems are large decentralized nonlinear systems. Because of the growing ecological pressure and the necessity to implement more renewable sources like wind turbine generators as well as new technologies like fuel cells into the system its dynamical behavior changes to be more difficult. The deregulation and liberalization of the electricity market forces a reduction of overcapacities and reduces the investments into the net. Consequently the power systems run closer to their physical stability limits than ever before. Different phenomena like “swing” and “collapse” incidents can already be detected.

Technologies like FACTS–Devices (Flexible AC Transmission System) can help to overcome some problems. To implement such devices or to determine a suitable control strategy to steer the power system sophisticated analysis of dynamical properties is necessary. The dynamical behavior of power systems is determined by load characteristics, mainly. Due to the large amount of different loads, the characteristics are analyzed in the past by simulational studies based on time series analysis, mainly. The influence of the load characteristics on the principal dynamics of the electric power systems are known for some special cases, only.

One possibility to analyze the dynamics in a structured way and to overcome the disadvantages of time series analysis, is to apply continuation methods, to calculate all possible solutions of a power system under study. The application of continuation methods in power system analysis and computation of dynamics has the advantage, that beside a possible time series calculation, the complete solution of the system in dependence of interesting parameters can be achieved. Furthermore, sophisticated software programs can classify the properties every calculated solution point has. Special interesting bifurcational properties can be continued. So called bifurcation diagrams can be computed. Bifurcation diagrams show the system behavior in dependence on a continuation of parameters. Characteristic points where the system changes its behavior are called bifurcation points or short bifurcations.

In the past several load models are presented. Only some of them represents the load in a physical relevant way and hence can be used for structural analysis. An often used model is presented and implemented in a representative three node system. Although this model considers different system states, it neglects the dependency of the reactive load demand on a deviation of the node voltage. Another load model which implement inter alia the mentioned dependency is presented. This paper integrates the model in the representative three node system in order to realize the influences on the power system dynamics of load characteristics. The different characteristics are represented by parameter changes.

Several characteristic results of bifurcational analysis if load parameters are varied in a structured way are presented. All results will be interpreted physically. Based on the calculated solutions further investigation can result in concepts to prevent critical system states by matched bifurcational control strategies. An outlook is given, how to combine bifurcational control of power system dynamics with realized control tasks.

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A Study of Mathematical Model of Piezoelectric Transducer on Energy-Recycling Semi-Active Vibration Suppression

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An energy-recycling method enables effective semi-active vibration suppression with piezoelectric transducers. With this method, the energy is collected from the mechanical energy of a vibrating structure, and stored in the capacitor of a piezoelectric transducer as an electric charge, and then used for vibration suppression rather than simply dissipated. This energy-recycling idea is called LR-switching method, whereas the conventional semi-active method is called R-switching. These methods supply no energy to the system, which means that the system is always stable. This LR-switching method based on energy-recycling approach for vibration suppression is surely attractive not only for general mechanical structures but also for special structures with limited or even no source of energy, such as space structures.

In this paper, first, the vibration control utilizing the new energy-recycling method is discussed. Then formulae that describe the behavior of structure and electricity, and several control strategies on the basis of active control theories for this method are presented(Fig.1). In addition, we show an advanced electric circuit using diodes for simplifying the control law and reducing the hardship of measurement on an actual control system. This energy-recycling semi-active method is designed for multiple-mode vibration suppression with multiple transducers, because target values obtained from active control theories are used. To see whether the energy-recycling method works in an actual structure, an experiment of vibration suppression of a truss was performed using both the energy-recycling LR-switching method and the R-switching method. Through numerical simulations with mathematical model of piezoelectric transducer and experiments, the new method is shown to be more effective in suppressing vibration than both the conventional semi-active method and the optimally tuned passive system. However, there were some discrepancies between the experimental results and the numerical results with ideal linear characteristics of the piezoelectric transducers estimated from a static test. Therefore we investigated the differences between actual behavior and ideal condition on the numerical simulation. With some adjustments on the mathematical model, the numerical result agrees with the experimental result(Fig.2).

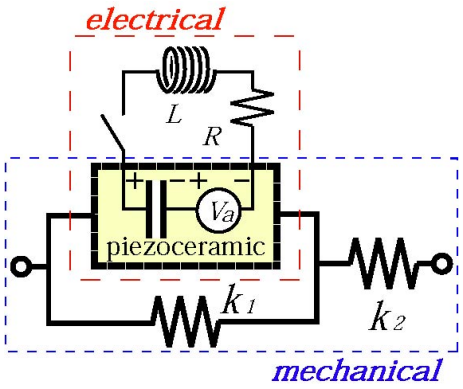

Figure 1: An electric circuit for the energy-recycling semi-active method and a model of piezoelectric transducer

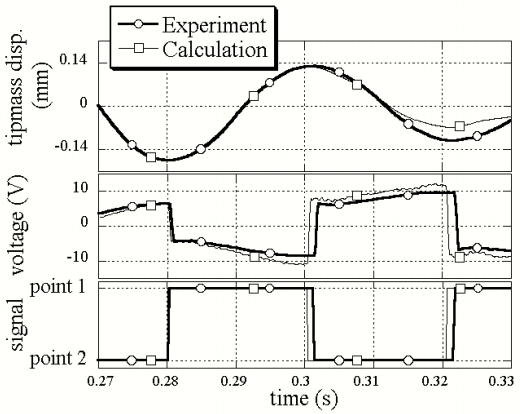

Figure 2: Numerical result and experimental result with the energy-recycling semi-active method

MULTI-LEVEL MODELLING OF A MODULAR DOUBLE SALIENT LINEAR MOTOR

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The three-phase modular double salient linear motor is a direct-driven linear motor, which can replace rotational to linear movement translator devices. Due to its modular construction the motor is simple, efficient and has high positioning accuracy. Therefore it is ideal for applications that require high position accuracy and repeatability.
The multi-level model of this motor couples several units implemented using different simulation platforms (SIMULINK, SIMPLORER and MagNet), each being one of the bests in its field. Hence the main advantages of each one was exploited and the global efficiency of the entire simulation program is as high as possible.

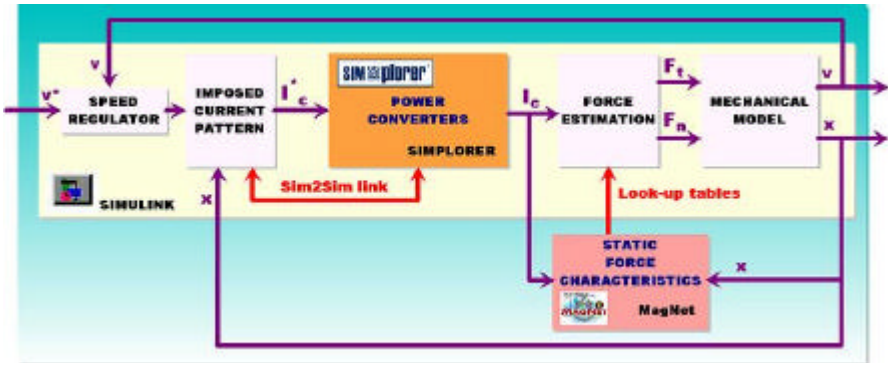

Fig. 1. The block diagram of the coupled simulation program

The basis of the whole model is the motor's MATLAB/SIMULINK unit. It exploits all the benefits of MATLAB (easy to write program lines, advanced graphical visualisations) and of SIMULINK (simple modular model building, easy to use graphical interface, etc.). The field computations were made using MagNet 6.0 FEM-based magnetic field analysis program. The obtained results, the static characteristics of the forces, were integrated in the SIMULINK model by easy-to-use look-up tables. The power converter's model was made in SIMPLORER, a widely used simulation program in the field of power electronics. The converter units were coupled into SIMULINK by the Sim2Sim link. This way all the parts of the model were implemented in the most suitable platform for each of them.
All the obtained results are in good accordance with the theoretical expectations and with the results of analytical computations. This means that the overall performances of the combined simulation program are quite good. Therefore the idea of coupling units built-up in different simulation platforms into a single simulation program could be also used for simulating similar types of electrical machines.

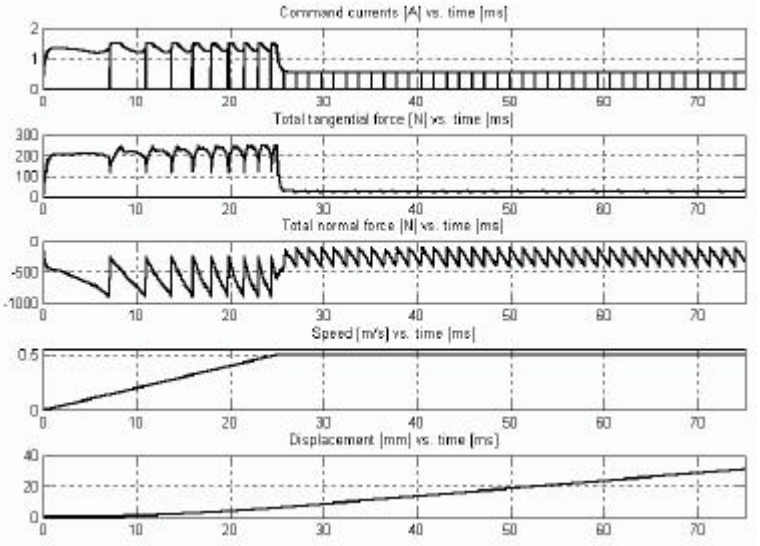

Fig. 2. Results of simulating the starting of the motor

COMPUTATION OF NONLINEAR RESONANCES OF SATURATED SYNCHRONOUS MACHINES CONNECTED TO AN INFINITE BUS BAR

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An important model in power system engineering is that of a nonlinear synchronous machine connected to an inifinite bus bar. Very often an idealized model for the machine is used, where all flux densities are assumed to be proportional to the currents. Therefore magnetic saturation or other nonlinear effects can't be treated. But, which is well known from practice, saturation has a great influence to the machine's behavior and much ingenuity has been used in devising methods of taking it into account; for example, the use of 'Potier reactance'. Such methods do not, however, introduce the nonlinear property into the basic theory. They are directed mainly to the determination of appropriate values of constants to suit the particular problem, the constants being defined in relation to a linear theory.

In this paper a nonlinear model of the machine is used, which allows to study the effects of the nonlinearities in a very structured manner. The models are in such a shape, that they can be handled mathematically in an efficient way. It is not the goal to fit all measured points of a e.g. saturation curve in detail, but we are interested in the typical behavior and the influence of important nonlinear effects on the dynamics of the system.

An analytical solution of those nonlinear systems is reachable for some cases, only. With the help of differential geometry statements on particular properties can be made. Equilibria and their description on manifolds of equilibria are sophisticated tools for analysis. Critical equilibria, which denotes to a structural change in solvability and therefore to quite different solutions of the system, can be analyzed. In particular, if one is interested in to know, if the system can reach such critical points and may be reach different forms of stability or instability, even in a dynamical case.

The emphasis of this paper is focused on the calcuation of nonlinear resonance phenomena, when a synchronous machine is interconnected to an infinite bus bar or in a second case for interconnected machines. For different frequency ranges, simulations where performed to show the resonance effects. From an application of catastrophe theory and analytical analysis on this system it is known, that the system will reach some bifurcational points, especially a synchronous machine will undergo some hopf bifurcations to reach a cusp bifurcation. In our simulational studies which were done by the help of the MATLAB package, the effect of the cusp will be shown, the problems in simulating such nonlinear systems in the presence of a cusp bifurcation by time series analysis is discussed.

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COMPUTATION AND ANALYSIS OF HYSTERESIS EFFECTS BY APPLICATION OF DEFORMATION METHODS

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Extended Abstract. Electrical power system are in a global change. Due to liberalization or the need for more efficiency of the nets, power systems are forced to be operated closer to their stability margins. Nonlinear effects can be observed much more than in the past, the characteristics of the systems become more and more nonlinear. From this, there is a need in even more detailed models of the elements in such a form, that nonlinear analysis can be done efficiently. Importend for this task is, that not some special system elements are analysed for themselves or some time intervals only, since in this case the structural properties of the complete system will be lost. Obviously, there is a need for models are which preserves the structural properties to describe the nonlinear dynamics properly.

Unefficient numerical computational methods leads to the lost of structural informations, often. Especially, stability analysis will be done in different kinds. Due to the nonlinear character of the power systems, methods based on linear theory are unsuitable, often. A complete transition of the topological structure of trajectories in phase space due to a change of some control parameters are knows as bifurcations. The task of bifurcational analysis is to determine critical parameters which forces the system to a topological change and to determine and to construct the new solution branches. For this, special homotopy– and continuation methods are a suitable tool, to determine all structural and dynamical properties of a system under consideration. In this paper the structural properties of a hysteresis model for a single phase transformer will be discussed. The model is represented in a closed form. Simplifications of the model are made in the sense, that all stuctural properties are preserved, only.

In this paper it is shown, how a nonlinear differential representation of a transformer model with hysteresis effects can mathematically deformed to linear one with some additional nonlinear algebraic constraints. Therefore, the analysis of the new model is much more efficient, the bifurcational properties are preserved. Since the parameter of the hysteresis depends on magnetical properties of the core only, the influence of the core material on the dynamics of the system can be studied efficiently.

This kind of hysteresis modeling is motivated by practical problems. When power system dynamics must be analyzed or calculated with partly very old system components, for which no parameters are available, the classical modelling is no solution, since the approximated parameters are to bad for a use in practice. But material tables, characteristics of the core material is still available. Together with the characteric losses of transformers, an approximation of detailed dynamical properties can be achieved. The proposed model is used for educational tasks, also.

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Identification

A GRADIENT BASED METHOD FOR THE IDENTIFICATION OF HYBRID SYSTEMS

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The nature of hybrid systems is characterized by a strong coupling of their time driven and discrete event driven subsystems. For application issues these hybrid systems are often approximated by piecewise affine characteristic maps. This approach is widespread used in hybrid identification [1, 2].
For the determination of the parameters as well as their range of validity, least squares approaches can be applied to fit the given hybrid model structure to a set of measured data. Due to the discontinuities that may appear in hybrid systems, this results in a nonlinear optimization problem. In [3] it was shown that this optimization problem is even discontinuous. As a consequence, standard numerical gradient based routines cannot be applied immediately to solve this minimization.
The methods proposed in [1, 2] try to solve this optimization problem approximately by applying clustering techniques to determine the different subdomains. The high computational effort is due to the extensive number of affine estimates calculated for the determination of these domains.

To overcome these problems and to determine the parameters of hybrid systems with piecewise affine dynamics, the proposed approach transforms the hybrid identification problem into a continuously differentiable optimization problem by using suitable approximations.
It turns out, that the step–functions used to fade in and out the different affine submodels cause the discontinuities in the optimization problem and hence, these functions are replaced by continuously differentiable functions. The requirements on the approximations are discussed and the corresponding necessary and sufficient conditions on the approximations are obtained.
Since standard optimization software can now be applied to solve the resulting optimization problem, it becomes obvious that the complexity of the hybrid identification problem is reduced significantly. For a further reduction of the computational burden an approximative algorithmic solution of the optimization is proposed:

- In the first step, only hypercuboidal domains are permitted for the submodels. By applying optimization tools, the configuration of these partitions is optimized such that a quadratic performance index is minimized.
- Since the resulting partitions are hypercuboids, the corresponding vertices do not reflect the optimal positions of the affine models; thus in a second step the positions of the partitions' vertices are optimized to achieve higher precision of the identified model.

The reduction of the computational complexity in the first step is based on the reduced number of parameters compared to the case in which partitions of arbitrary shapes are permitted. Optimizing the partitions' vertices in the second step is done by shifting the vertices only in a locally bounded domain and hence the computational complexity is kept low again.
The different steps of the identification procedure are demonstrated at a multidimensional hybrid characteristic map.

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DYNAMIC SYSTEMS IDENTIFICATION WITH GAUSSIAN PROCESSES

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Most control engineering applications are still based on parametric models, where the functional form is fully described by a finite number of parameters. The information about uncertainty is usually expressed as uncertainty of parameters and do not take into account uncertainty about model structure, or distance of current prediction point from training data used to estimate parameters. This paper describes modelling based on Gaussian processes which is an example of a non-parametric model that gives also the information about prediction uncertainties which are difficult to evaluate appropriately in nonlinear parametric models. Gaussian processes approaches which originated in statistics research are in many respects related to artificial neural networks, in terms of their application domain. It was shown that neural networks and Gaussian processes were closely related, even more, in the limit of an infinite number of neurons in hidden layer the two are equivalent. Nevertheless, majority of work on Gaussian processes shown up to now considers modelling of static non-linearities. Fragments on the use of Gaussian processes in modelling dynamic systems have been published recently, e.g. [2,3] and propagating of variance in dynamic system has just been revealed [1]. Bringing all this contributions together would show all the aspect of dynamic systems identification by means of Gaussian process models which is the purpose of this paper. A Gaussian process is an example of the use of a flexible non-parametric model with uncertainty predictions.

Gaussian process is a collection of random variables which have a joint multivariate Gaussian distribution. Assuming a relationship of the form $y = f(x)$ between the inputs x and outputs y, we have $\mathrm{Cov}(y^p, y^q) = C(x^p, x^q)$, where $C(.,.)$ is some function with the property that it generates a positive definite covariance matrix. This means that the covariance between the variables that represent the outputs for cases number p and q is a function of the inputs corresponding to the same cases p and q. Given a set of training cases , the hyperparameters of the covariance function should be learned. There is a hyperparameter correponding to each regressor 'component' so that, after the learning, if a hyperparameter is zero or near zero it means that the corresponding regressor 'component' has little impact so could be removed. Gaussian processes are, as neural networks, approximators of static nonlinearities and can therefore be used for modelling of dynamic systems if delayed input and output signals are fed back and used as regressors. In the framework of Gaussian processes, k-step ahead prediction can be achieved by simulating the system (repeated one-step ahead predictions up to k - *iterative method*). The described approach is illustrated with identification of system that can be described with equation $\dot{y} = -\tanh(y + u^3)$. The output signal was disturbed with white noise. Results on validation signal, different from the identification one, show that Gaussian process model successfully models the system based on chosen identification signals. Moreover the information about uncertainty which comes with the Gaussian process model indicate the level to which results are to be trusted.

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Identification of Optimal Mathematical Model of External Impacts

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At mathematical modeling of real motion of open dynamic systems is important the correct choice of mathematical model of external impact on system. This impact is little-known as a rule. In many cases the well investigated external impact is consider as external known impact with goal to obtain more simple description of dynamic system. We shall suppose for simplicity that with the aid of known internal interactions (for example, measured experimentally) some subsystem of initial dynamic system can be received at which is known one variable status and all external impacts except impact which is being investigated.
A problem of the finding of scalar function of external impact z(t) in many cases can be reduced to the solution of the linear integral equation Vollterra of the first kind

$$A_{\bar{p}} z = u_\delta,\ z \in Z,\ u_\delta \in U; \qquad (1)$$

where Z,U are B functional spaces, $A_{\bar{p}} : Z \to U$ is compact integral operator [2] and one depends on vector-parameters of mathematical model $\bar{p} = (p_1, p_2, \ldots p_m)^*$, $\bar{p} \in R^m$. It is supposed that the parameters of mathematical model are determined inexact with some error and by virtue of it they can accept values in known limits $p_i^0 \le p_i \le \hat{p}_i$ i = 1,2,3, ... , m. Therefore, the vector-parameters $\bar{p}$ had not defined precisely and that it can accept values in some closed area $\bar{p} \in \bar{D} \subset R^m$. The operator $A_{\bar{p}}$ in (1) will correspond to everyone of vector-parameter $\bar{p} \in \bar{D}$ and they form some class of operators $K_A = \{A_{\bar{p}}\}$. The function u_δ is obtained from experiment with a known error δ: $\| u_T - u_\delta \|_U \le \delta$, where u_T is an exact response of object on real external impact. We denote by $Q_{\delta,\bar{p}}$ the set of functions which satisfy the equation (1) with the exactness of experimental measurements at the fixed operator $A_{\bar{p}}$:

$$Q_{\delta,\bar{p}} = \{ z : z \in Z,\ \| A_{\bar{p}} z - \bar{u_\delta} \|_U \le \delta \}. \qquad (2)$$

The set of $Q_{\delta,\bar{p}}$ is unbounded set in norm of space U [2]. Any function from $Q_{\delta,\bar{p}}$ is the good mathematical model of external impact. However not all of them are convenient for further use in mathematical modeling. Let the value some continuous non-negative functional $\Omega[z]$, defined on Z_1 (Z_1 is everywhere dense set in *Z*) characterizes a degree of functions convenience from the set $Q_{\delta,\bar{p}}$. Let the function $z_{\bar{p}} \in Q_{\delta;\bar{p}}$ satisfies the condition:

$$\Omega[z_{\bar{p}}] = \inf_{z \in Q_{\delta;\bar{p}} \cap Z_1} \Omega[z]. \qquad (3)$$

Furthermore there are no bases to believe that the function $z_{\bar{p}}$ will be close to real external impact. It is only "good" and convenient model of external impact.
Let's consider new problem of construction (synthesis) of model of external impact $z^{opt} \in Z_1$ which provides the best results of mathematical modeling uniformly for all operators $A_{\bar{p}} \in K_A$:

$$\| A_{\bar{p}} z^{opt} - u_\delta \|_U \le \inf_{z_{\bar{p}}} \sup_{A_{\bar{p}_\alpha} \in K_A} \| A_{\bar{p}_\alpha} z_{\bar{p}} - u_\delta \|_U \ \text{ for all } A_{\bar{p}} \in K_A. \qquad (4)$$

Let us name function z^{opt} as *optimal mathematical model of external impact for all class K_A*. The possible algorithm of construction of function z^{opt} is offered in this work. The calculation of model of external impact for rolling mills was executed.
The offered approach to synthesis of optimal mathematical models of external impacts on dynamical system can find application in cases when the information about external impacts is absent or poor and also with check of hypotheses on the basis of which were constructed the known models.

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Modelling in Mechatronics
Methods and Applications

Symbolic Differential Elimination for Symmetry Analysis[1]

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Differential problems are ubiquitous in mathematical modeling of physical and scientific problems. Algebraic analysis of differential systems can help in determining qualitative and quantitative properties of solutions of such systems. We describe several algebraic methods for investigating differential systems.

The idea of an algebraic approach to differential equations has a long history. In the 19th century S. Lie initiated the investigation of the group of transformations leaving a given differential equation invariant. This group is used to reduce the order or the number of variables appearing in the equation. Lie discovered that knowledge of a one-parameter group of symmetries reduces the order of an ODE by one.

At the beginning of the 20th century Riquier and Janet introduced involutive bases of differential polynomials. These are canonical systems of ideal generators which can be found algorithmically similar to Buchberger's well known Gröbner basis algorithm. Computing these Janet bases for Lie symmetries of a differential equation, triangularizes the determining system.

There are several advantages of an algebraic analysis of differential equations:

- sometimes we may actually find a symbolic solution;
- deriving symmetries may help in verifying numerical schemes for approximation of solutions;
- we can decide whether a system of ODEs or PDEs admits a solution,
- if there are solutions, then we can derive equivalent triangulized systems;
- we can get a complete overview of the algebraic relations satisfied by the solutions system of differential algebraic equations.

An effective symbolic treatment of differential problems depends crucially on algorithms in differential elimination theory. The algebraic theory of elimination is well developed, and we can answer constructively the main questions like membership, radical membership etc. The methods for solving these problems are resultants, Gröbner bases, and algebraic involutive bases. For differential ideals there are still many open problems. For instance, the membership problem or the ideal inclusion problem for finitely generated differential ideals are still not solved.

There are several approaches to the field of differential elimination. In this paper we concentrate on differential Gröbner bases, involutive bases, characteristic sets, and symmetry analysis.

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IDENTIFICATION OF LINEAR ERROR-MODELS WITH PROJECTED DYNAMICAL SYSTEMS

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Linear Error-models are an integral part of several parameter identification methods for feedforward and feedback control systems. The parameters are hereby often subject to specific restrictions, which span convex solution sets. The reason for these restrictions is for example the demand for invertibility of a static nonlinearity during a synthesis of an inverse feedforward controller [1] or the demand for stability of a feedback control system during the synthesis of a respective controller [2]. If the restrictions can be formulated through inequality constraints the admissible solution set for the parameters is a convex polyhedron and the corresponding identification problem to be solved is a convex quadratic program. For solving these well conditioned problems before putting the control system into operation the optimisation theory provides multiple powerful algorithms. But these algorithms are not suitable for an optimisation during the operation of the control system, because they require too much computing power. A possibility to avoid these difficulties is to formulate the solution of the bounded quadratic optimisation problem as a stable equilibrium point of a proper system of differential equations. This dynamical system can then be solved through numerical integration very efficiently from time step to time step during the operation of the control system. In the unbounded case, for instance, the right-hand side of the demanded differential equation is given by the negative gradient of the quadratic target function. The theory of the projected dynamical systems [3] offers a starting point for the formulation of a respective differential equation for the bounded case. In this case the vector field of the differential equation is also based on the negative gradient of the quadratic target function. However, the right-hand side of the differential equation follows in this case from a projection of the negative gradient which ensures that the trajectory of the system under no circumstances leaves the admissible solution set. In contrast to parameter projection methods normally used the in the field of adaptive systems, the applied projection transformation considers also the non-differentiability points of the boundaries of the convex solution set. As in the case of a convex polyhedron these non-differentiability points often result from the intersection of smooth convex sets. The projection transformation results in a discontinuous right-hand side of the differential equation. The consequence are difficulties for the verification of the existence, uniqueness and stability of a solution trajectory.
The main subject of this paper is the derivation of an alternative formulation of the projected dynamical system, which exhibits, in contrast to the original formulation, a continuous right-hand side and thus is accessible to conventional analysis methods. For this purpose the multi-dimensional stop operator, well-known from the hysteretic systems theory, is used [4,5]. Finally the existence and uniqueness of the solution trajectories are verified and the stability properties of the projected dynamical system are investigated.

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MODELING AND FLATNESS-BASED FEASIBILITY STUDIES FOR ELECTRO-MECHANICAL BRAKE-BY-WIRE ACTUATORS

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Electro-mechanical brake-by-wire (EMB) actuators are usually made up of a standard disc brake, a roller or ball screw and a brushless electric machine with optional gear reduction [1]. Due to their reliability switched reluctance (SR), brushless DC (BLDC), and squirrel cage induction machines (IM) are considered as the most likely candidates for the electric drive of the EMB actuator.
A crucial point in the design of such EMB actuators is to meet the dynamic requirements w.r.t. position x of the brake pads or the clamping force F_c of the disc brake, resp., without violating technical input and state constraints. From a control engineering point of view, the actuator operation represents a nonlinear tracking problem for the reference variable, *i.e.,* $x(t)$ or $F_\mathrm{c}(t)$, resp. Thus, the controller design comprises two steps: At first, a suitable reference trajectory $x^\mathrm{d}(t)$ or $F_\mathrm{c}^\mathrm{d}(t)$ has to be specified according to the most challenging dynamic requirements. Secondly, open or closed loop controllers can be designed that steer the system along the reference trajectory. Therewith, the fulfillment of system variable constraints has to be verified in order to estimate the feasibility of a particular actuator w.r.t. dynamic specifications.
A systematic solution of the tracking problem for nonlinear systems is possible using the inverse system approach based on the differential flatness [2,3,4]. The inverse system is purely algebraic and allows the examination of the system constraints without performing simulations. Of course, the flatness approach requires mathematical models for the actuator components. Thus, Section 2 of this contribution is devoted to the modeling of the considered family of EMB actuators, which comprise BLDC, SR, and IM machines for the electric drive and a general representation of the actuator's mechanics. The modeling of the mechanics is exemplified in Section 3 by means of a ball screw. Based on the presented model, the flatness of EMB actuators is shown in Section 4. Finally, trajectory planning and flatness-based design of an open loop control are performed for a SR machine, in order to illustrate the approach for the flatness-based feasibility study. In doing so, it turns out that the considered SR machine does not fulfill the dynamic requirements of an EMB actuator, because input constraints are violated.

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THE AUTONOMOUS WHEELCHAIR "EASY" AND ITS HIERARCHICAL CONTROL

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Robots acting in the proximity of humans belong to the most challenging mechatronic systems and attract increasing interest in sciences and in commercial applications. The autonomous wheelchair EASY (electric wheelchair with driver assistance system) is an example of such a system of high autonomy and is developed in the author's research group. This contribution introduces the hierarchical control structure of the system and particularly focuses on two feedback control tasks: (i), the problem of trajectory tracking of the non-holonomic system is solved using a flatness based feedback design, and (ii), for the camera supported control of path segments an approach of image-based visual servoing is introduced. Here, the application of a 3D laser supported camera allows for precise positioning using a 3D state-feedback algorithm.

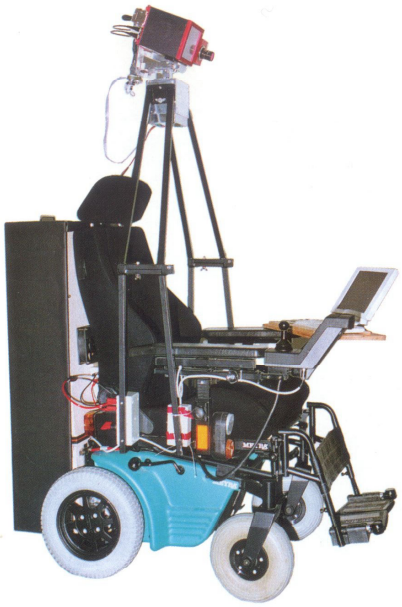

Fig. 1: Wheelchair with camera, computer, and user interface

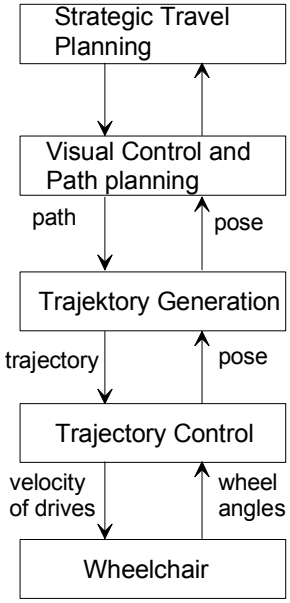

Fig. 2: Hierarchical control

Fig. 2 shows the (simplified) hierarchical structure of the different control loops: On the two lower levels, the trajectory generation and trajectory tracking are done, which rely on measuing by incremental encoders installed in the rear wheels. The visual control and path planning is based on evaluating the images of the 3D camera. On the one hand, this can be supported by artificial landmarks; on the other hand, obstacles must spontaneously be avoided by additional measures. On the level of strategic travel planning, the human keeps the upper hand, by giving travel goals and by intervening if necessary.

1) *Flatness Based Trajectory Tracking Control*: If a dynamic system is *differentially flat*, then it is possible to calculate the trajectories of the state variables and of the control input variables from a given trajectory of the so-called flat output, without numerical integration. The resulting relations make a particularly simple feedback control design possible, with the goals of stabilizing the system and ensuring trajectory tracking.

2) *3D Image-Based Visual Servoing*: The block "trajectory generation" frequently requires intermediate reference goal poses as an input. Such goal poses can be calculated by using image data from a camera and by determining the next part path to be followed. In order to do so, the the current images from the camera are compared to corresponding images taken during a teaching drive. From this comparison, goal poses can directly be generated and be used as the reference input signals to the trajectory generation, resulting in an image-based closed-loop (fig. 3).

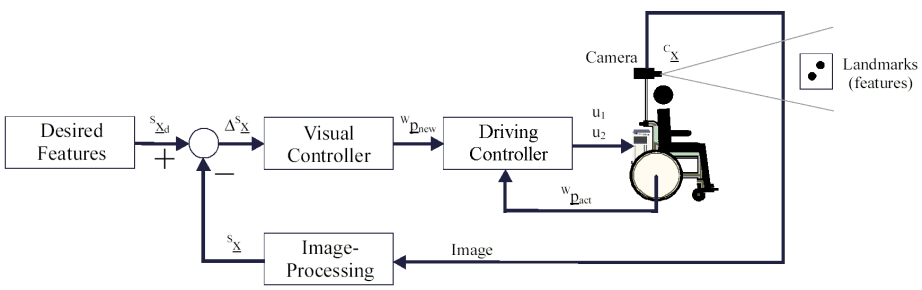

Fig. 3 Visual Servoing feedback control loop

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Modelling in Mechatronics
Multiport Modelling of Physical Systems

ENERGY BASED MODELLING OF LUMPED-PARAMETER HYDRAULIC SYSTEMS

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The energy based modelling of nonlinear systems was mainly stimulated by the demands on the controller design for dynamical systems where the nonlinear components cannot be neglected. In this context, modelling turns out to play a central role within the control system design. By modelling, we not only mean the process of setting up the equations for simulation purposes but also the process of revealing the structural aspects of the system which, in a further step, can be exploited for the controller design. The most popular control design strategies based on this philosophy are involved with the fundamental notions passivity and dissipativity. In the literature, passivity-based control and energy based modelling can be found in a wide range of applications, see, e.g., [2], [4], [6]. Nevertheless, as far as the authors know, lumped-parameter hydraulic actuators have not yet been considered within this world. Even though in e.g., [7], the more complicated infinite-dimensional case of a fluid dynamical system was already modelled as a Hamiltonian boundary control system.

This is why, in this paper, we concentrate on a systematic derivation of an energy based description of lumped-parameter hydraulic actuators. In this context, the modelling in the form of a port-controlled Hamiltonian system with dissipation or PCHD-system for short, see, e.g., [6], offers a pleasing way to describe the structural aspects of the energy storage mechanism and the energy flows to and off the system due to external inputs. In a first step, a systematic formulation of the constitutive relations of a fluid in an isentropic process, e.g., [1], [5], beginning with the fundamental laws of thermodynamics, is given. We further show that the definition of the bulk modulus, usually used as a constitutive law in industrial hydraulics, fits this description. As an additional result, we are able to formulate a coenergy principle for calculating the generalized coupling forces of hydraulic actuators in complete analogy to electromechanical systems. These results allow us to describe the hydraulic systems under consideration in the same mathematical framework as we are used to for electromechanical systems. It is worth mentioning that, in contrast to the equivalent electric circuit models of lumped-parameter hydraulic systems, see, e.g., [3], the theory presented is not confined to the linearized scenario. Thus, we will also show that the definition of a "hydraulic capacitance" as a fluid element in which potential energy is stored may lead to a wrong interpretation, if used in an energy based modelling context.

As a result, we will present the PCHD-model for a general configuration of a translational hydraulic piston actuator with an isentropic fluid. It turns out that the PCHD-system has two non-trivial dynamical invariants, so called Casimir functions, if the dissipative effects in the hydraulic part (leakage flows) are neglected. These observations together with the analogy to electromechanical systems give us the necessary information for the choice of suitable canonical coordinates.

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Distributed Port Hamiltonian Formulation of the Timoshenko Beam: Modeling and Control

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Abstract

The purpose of this paper is to show how the Timoshenko beam can be fruitfully treated within the framework of distributed port Hamiltonian systems (dpH systems), both for modeling and control purposes. In this manner, rather simple and elegant considerations can be drawn regarding both the modeling and control of this mechanical system. In particular, it is shown how control approaches already presented in the literature can be elegantly uni ed, and a new control methodology is presented and discussed.

The paper is organized as follows: rst of all, the dpH model of the Timoshenko beam is presented and the underling *Dirac structure*, the core of the Hamiltonian structure of the model itself, is shown. Then, some considerations about several control strategies of the beam are presented. In particular, the well-known control by *damping injection* is extended to distributed parameter systems in order to stabilize the beam acting through its boundary and/or its distributed port. Moreover, the *energy shaping* by interconnection control technique is extended to distributed parameter systems in order to control a mechanical system made of a exible beam with a mass connected at an extremity. The nite dimensional controller, acting on the system through the other extremity, is developed by properly extending the concept of *Casimir functions* to the in nite dimensional case.

Finally some conclusions and ideas for future work are presented.

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A NOVEL PASSIVITY PROPERTY OF NONLINEAR RLC CIRCUITS*

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Passivity is a fundamental property of dynamical systems that constitutes a cornerstone for many major developments in circuit and systems theory, see e.g. [4] and the references therein. It is well-known that (possibly nonlinear) RLC circuits consisting of arbitrary interconnections of passive resistors, inductors, capacitors and voltage and/or current sources are also passive with port variables the external source voltages and currents, and storage function the total stored energy [2].

Our main contribution in this paper is the proof that for all RL or RC circuits, and a class of RLC circuits (with convex energy function and weak electromagnetic coupling) it is possible to 'add a differentiation' to the port variables (either voltage or current) preserving passivity with a storage function which is directly related to the circuit power. The new passivity property is of interest in circuit theory, but also has applications in control. To establish our results we exploit the geometric property that voltages and currents in RLC circuits live in orthogonal spaces, i.e., Tellegen's theorem [2, 3], and heavily rely on the seminal paper of Brayton and Moser [1] published in the early sixties.

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DYNAMIC MODELLING OF MECHATRONIC MULTIBODY SYSTEMS WITH SYMBOLIC COMPUTING AND LINEAR GRAPH THEORY

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Linear graph theory, invented by Leonhard Euler in 1736, was applied to the modelling and analysis of one-dimensional physical systems in the 1950s and 1960s [1]. The basic theory of this modelling approach was established during this period, and subsystem analysis methods were developed for large electrical networks [2]. Quite recently, graph-theoretic methods for modelling flexible multibody systems were developed [4], an overview of which is presented in the paper. Graph theory can be used to generate equations in terms of user-selected coordinates, including absolute or joint coordinates, or some combination of the two. By selecting coordinates that are well-suited to a given problem, one can reduce the number and complexity of the governing equations.
Given that linear graphs were originally applied to electrical networks, the extension of graph-theoretic methods to the modelling of mechatronic multibody systems is natural and straightforward. From a single linear graph of the entire system, the coupled equations for the electrical and mechanical subsystems are systematically derived. Symbolic programming was used to implement this graph-theoretic formulation; the resulting Maple program (DynaFlex) for modelling flexible multibody mechatronic systems is briefly described.

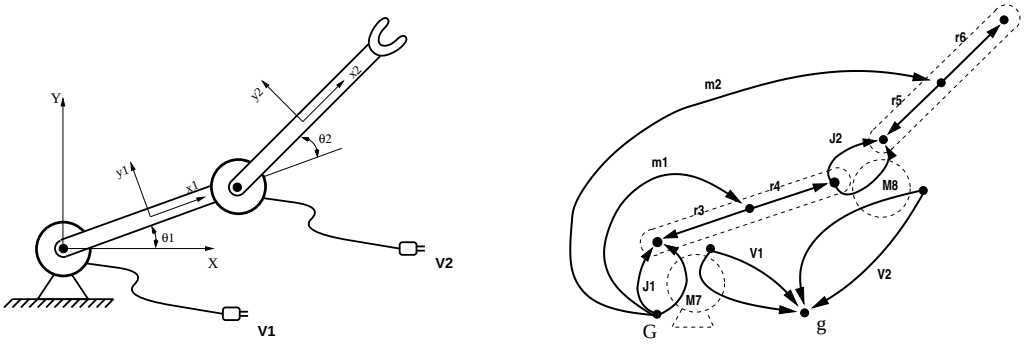

Figure 1: DC motor-driven robot manipulator and linear graph.

To demonstrate, consider the two-link manipulator shown in Figure 1 with its linear graph representation. The joint angles θ_1 and θ_2 are controlled by two DC motors that are powered by voltage sources V_1 and V_2. The linear graph of the system contains the standard mechanical components, the two voltage sources, and the two motors M_7 and M_8. Four differential equations, in terms of θ_1, θ_2, and the two motor currents, are generated for the two-link manipulator. These system equations can be used to find symbolic inverse solutions for the motor currents required to drive a particular trajectory, or as the basis of a forward dynamic simulation [3].
The modelling of complex systems is greatly facilitated by the use of subsystem models; a newly-developed graph-theoretic generalization of the Norton and Thevenin theorems from electrical network theory is used to generate models of mechanical and electrical subsystems, from which a multibody mechatronic system model is constructed. The utility of this subsystem modelling approach is demonstrated on a PD-controlled robot arm.

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NETWORK MODELLING OF A CLASS OF ACOUSTIC SURFACE WAVE FILTERS

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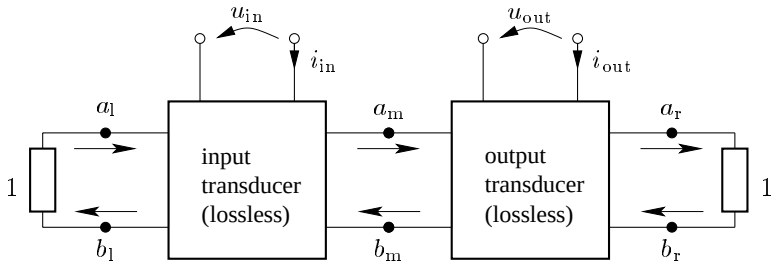
The paper presents a detailed analytical description of a wide class of surface acoustic wave (SAW) filters built by cascading two electro-acoustic transducers as shown in the figure. Unlike classical FIR design for SAW filters the introduction of internal reflections in the transducers offers new and extremely promising possibilities of true rational transfer function design for SAW filters [1]. Due to the internal absorbers (unit resitances in the figure) the filters, as viewed between the two external electrical ports, are inherently lossy devices that present themselves in a natural manner as the Darlington embedding of a lossy two-port into a lossless four-port.



The most natural parameterization of SAW transducers is in terms of the so-called P-matrix of the 4-port — a *mixed* matrix representation that relates the 2-vectors of voltages u and currents i of the external electrical ports and the 2-vectors a and b of the acoustic wave variables at the internal absorbers by

$$\left[\begin{array}{c} i \\ \hdashline b \end{array}\right] = \left[\begin{array}{c:c} C & R \\ \hdashline L & B \end{array}\right] \left[\begin{array}{c} u \\ \hdashline a \end{array}\right], \quad \text{where} \quad P(z) = \left[\begin{array}{c:c} C(z) & R(z) \\ \hdashline L(z) & B(z) \end{array}\right] \quad \text{is a rational } (4 \times 4) \text{ matrix over the unit disk.}$$

In [2] we analysed the general algebraic and analytic properties of the P-matrices of lossless and reciprocal multiports by establishing their intrinsic connection to the Arov-Dewilde-Dym parametrization of J-inner functions [3]. More in detail, in the present paper we show that the transducer 3-ports are very naturally decribed as a cascade connection of various sections that serve as network models for the *excitation*, *reflection* and *propagation* of the acoustic waves, where the structural "backbone" of the SAW-filter is formed by a resistively terminated transmission line transformer. We establish $P(z)$ formally as a linear fractional transform

$$P(z) = \mathcal{F}_{\mathbf{\Pi}}(P_0) = A + BP_0(1_{h+d} + DP_0)^{-1}C, \qquad \text{where} \quad P_0 \in \mathbb{R}^{4\times 4}$$

and $\mathbf{\Pi} = \mathbf{\Pi}(z)$ is a rational (8×8)-matrix that results from the Redheffer product of certain elementary matrices. By application of the reactance extraction approach, finally, we end up with the state space representations of $P(z)$ as well as its submatrices, especially the (2×2) admittance matrix $C(z)$ of the electrical filter (a Carathéodory function) and the Blaschke matrix $B(z)$ of the internal transmission line transformer. Furthermore, we show that the representation is unique, i.e., the lossless cascade structure pins down the related spectral factorization problem to a unique solution.

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TERMINAL BEHAVIOUR OF NETWORKS, MULTIPOLES AND MULTIPORTS

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The theory of terminal behaviour is one of the central parts of network theory. Together with its closely relatives, network synthesis and network modelling, it builds the bridge between network theory as pure mathematical discipline and the applications of network theory in physics, engineering, etc. Moreover, the theory of terminal behaviour characterize the limitations of the modelling capability of networks. Many wellknown theorems of network theory describe properties of the terminal behaviour of networks, e.g., the theorem on Δ-Y-transformation, the source shifting theorems going back to BLAKESLEY, the theorems of THÉVENIN and NORTON, and many others. The methods of diacoptial analysis of large-scaled circuits are justified also by means of the theory of terminal behaviour. The definition of the notions of multipoles and multiports given in almost all standard textbooks are indeed very weak. Difficulties arise already by simple questions such as: Is each four-pole a two-port? What is really meant by an intrinsic four-pole or an intrinsic two-port? How much independent equations are necessary for a representation of the terminal behaviour of an n-pole or an n-port by means of a system of scalar behavioural equations?

Let $\mathcal{N}$ be a given network with a prescribed subset of its node set whose elements are denoted as terminals. The *terminal behaviour* of $\mathcal{N}$ has to characterize the behaviour of $\mathcal{N}$ with respect to all interconnections of its terminals with arbitrary admissible outer networks $\tilde{\mathcal{N}}$ in such a manner that if we replace the given network $\mathcal{N}$ in such an interconnection by means of an other network $\hat{\mathcal{N}}$ with the same terminal behaviour then we are unable to observe this exchange in all the outer networks $\tilde{\mathcal{N}}$ of these interconnections.

In applications we are frequently confronted with starlike interconnections of some central network $\mathcal{N}$ with a collection of satellite networks. Since we can consider such a set of satellite networks also as components of a unconnected outer network $\tilde{\mathcal{N}}$ this situation is simple generalization of that one mentioned above. The terminals of the components of the unconnected outer network $\tilde{\mathcal{N}}$ define now a partion of the terminal set of the central network $\mathcal{N}$ into terminal classes.

It can be shown that the terminal behaviour of each network can be represented by means of some special networks denoted as the *canonical representatives* of the terminal behaviour of the given network. The graphs of these canonical representatives are forests whose components are trees each of them connecting the terminals of one of the terminal classes of the given network. This observation motivates the definition of elementary multipoles and elementary multiports. The *elementary multipoles* and *multiports* are networks whose graphs are forests where for an elementary multiport these forests consist of only one-branch components. General multipoles and multiports are defined as networks whose terminal behaviour can be represented by means of some elementary multipoles or multiports, respectively.

An interesting problem in this connection is the question about the existence of elementary multipoles with a minimal number of branches representing the terminal behaviour of a given network. Some of the difficulties of classical four-pole theory mentioned above are closely related to this problem. As examples op-amp and transmission line models as well as the junction multiports of bond graph theory are considered.

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NONLINEAR STOCHASTIC CIRCUITS AND SYSTEMS – A GEOMETRIC APPROACH –

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Abstract.

Since around 1913 first nonlinear electrical circuits containing electronic tubes were developed by Meissner, Armstrong and others (see Mathis [1] for further details) the problem of noise became a main subject of circuit designers. In 1918 Schottky published a first fundamental paper where he investigated the physical aspects of thermal and shot noise. In 1928 thermal noise was studied in more details for linear time-invariant circuits by Johnson and Nyquist where the famous Johnson-Nyquist formula was derived using equilibrium thermodynamical arguments. Basically all these considerations applied the so-called Langevin approach that was developed by Langevin in 1908 for linear physical systems. A mathematical reasoning of the concept of Langevin can be given if the mathematical concepts of stochastic processes and stochastic differential equations are used. Although this approach became very successful in the analysis of noisy linear electrical circuits and systems it was observed by McDonald and van Kampen around 1957 that it runs into difficulties if one tries to formulate a noise description for certain nonlinear physical systems. The main problem behind these difficulties was that it is very essential to divide external and internal noise in physical systems. In the first case there are no problems because we have to transform in a nonlinear manner a stochastic process. In the latter case new physical aspects arise with respect to a physical interpretation of the results since in contrast to the first case the origin for deterministic behavior and the stochastic disturbance is the same. If e.g. an electrical current is considered we have a flow of quantized charges that are responsible for the deterministic as well as the stochastic behavior; the stochastic part cannot suppressed without a breakdown of the deterministic current. Fortunately internal noise can be described by external noise in the case of linear systems which is the reason why the Langevin approach is successful. If noisy nonlinear systems are studied it was pointed out by van Kampen that moments of different orders are coupled. As a consequence we cannot start with a deterministic description of a system and add the stochastic disturbance - just like in the linear case.
The paper is organized in the following manner. First we discuss some general aspects of physical dynamical systems. In the following section a theory for a large class of noisy nonlinear electrical circuits is presented. This theory was developed by Weiss and Mathis [3] during the last few years based on Stratonovich's concept of nonlinear nonequilibrium statistical thermodynamics [2]. Unfortunately the theory is restricted to so-called reciprocal circuits and therefore no gain circuit elements (transistors or tubes) can be included in a circuit under consideration. Especially noisy nonlinear oscillators cannot analyzed from this point of view. Therefore in the last section we will discuss some recent methods for analyzing stochastic differential equations published in the literature where e.g. bifurcations occur and therefore a geometric approach is useful.

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EFFICIENT INTEGRAL EQUATION MODELING WITH SEMISEPARABLE MATRICES

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Integral equations lead to semiseparable matrices when discretized. These are matrices of the type

$$A = (A_{i,j}),\ \text{where } A_{i,j} \in \mathbf{C}^{m_i \times m_j} \text{ satisfies } A_{i,j} = \begin{cases} D_i, & \text{if } i = j, \\ U_i W_{i+1} \cdots W_{j-1} V_j^H, & \text{if } j > i \\ P_i R_{i-1} \cdots R_{j+1} Q_j^H, & \text{if } j < i. \end{cases} \quad (1)$$

They are obtained e.g. when the kernel of the equation is split in a sum of separable components, a move that can always be made. In the early days of analysis of the semiseparable structure, the modeling was restricted to representations of the type $h(t,\tau) = \sum_i f_i(t) g_i(\tau)$, i.e. leading to models in which $W_i = I$ and $R_i = I$ for all i. The more general model we consider here puts the handling of semiseparable matrices squarely in the realm of time-varying system theory. This allows for a much greater modeling capability. In particular, we can use models with special numerical properties, such as consisting exclusively of orthogonal or unitary operations.
Semiseparable models are particularly useful when the number of terms in the model expansion is small. Such models can be named 'efficient'. Most of the classical operations done on models or matrices, such as inversion, QR or URV factorization are closed under 'efficient modeling'. For example, if A has an efficient model and $A = QR$, then both Q and R have efficient models that can be derived efficiently from the model of A. The basic theory for these operations is contained in the general theory for time-varying systems (which also considers infinite operators) as done in extenso in [1]. When specializing to matrices, even more can be gained by combining classical matrix techniques with system theoretical ideas, as is done e.g. in [2].
In the present paper we give a brief introduction to the main techniques (including an indication on how models can be obtained) and then move on to present a new result, namely how the Moore-Penrose inverse of a general operator can be obtained in an efficient fashion using operations on a model in a one-pass, top-down, left-to-right fashion. The complexity of the algorithm is as usual $n^2 N$ where n is the average complexity of the model and N the size of the matrix. It is hence linear in the size of the matrix when the model is efficient.

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A MAPLE PACKAGE FOR CALCULUS OF VARIATIONS BASED ON FIELD THEORY

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Already the antique scientists studied variational problems to find an optimal solution like the isoperimetric problem. Great interest in extremal problems has lead in the last centuries to the development of different variational problems in mathematics, physics or control. In addition, variational principles, like e.g. the Hamiltonian principles, open up new possibilities in mathematical physics or mathematical modelling, since they offer more insight into the structure of a problem. Therefore, it is often meaningful to study the Euler Lagrange equations even if their solutions do not coincide with the optimal solution of the variational problem belonging to them. It is well known that the derivation of these differential equations is often a lengthy and laborious task. Nevertheless one can fomalize this problem such that it becomes solvable by computer algebra methods.
This contribution presents a computer algebra package for Lagrangian systems, which allows to derive the differential equations and boundary conditions of the variational problem $\mathfrak{L}$ with Lagrangian given by

$$\mathfrak{L} = \int_{\mathcal{D}} l\left(x^i, u^\alpha, u^{(n)}\right) \mathrm{d}x^1 \wedge \ldots \wedge \mathrm{d}x^p.$$

The Lagrangian density l is a function of $p \geq 1$ independent variables $\left(x^i\right)$, $i = 1, \ldots, p$ and $q \geq 1$ dependent variables (u^α), $\alpha = 1, \ldots, q$ and may also depend on the partial derivatives $u^{(n)}$ up to the order $n > 0$ of the dependent variables with respect to the independent ones. A solution, which meets the first variational formula of this problem, is called an extremal solution and they meet the famous Euler Lagrange equations. A well known method for the derivation of these equations is based on the so called Euler Lagrange differential operators δ_α. Since this approach makes heavy use of the so called integration by parts technique, it turns out that the derivation of the boundary conditions becomes a problem more complex than necessary. Therefore, this contribution proposes the use of the so called Cartan form. Having this form at one's disposal, one derives not only the Euler Lagrange equations but also the boundary conditions and certain first integrals in a straightforward manner. Furthermore, we show that the language of jet manifolds allows us to formulate the required relations and equations in such a precise and concise way that one can derive algorithms for a computer algebra system easily.
According to the remarks above, we give a short introduction to jet manifolds and summarize the results necessary for this contribution. Having the first variational formula at ours disposal, we discuss the construction of the so called Cartan form for three case. The first or ODE case with $p = 1$ involves one independent variable, whereas the second and the third case deals with $p > 1$ independent variables, where we have to distinguish between $n = 1$ and $n > 1$. Whereas in the first two cases the Cartan form is unambiguous and independent of the choice of the coordinates, one can construct several forms in the last case, but all of them generate the same set of differential equations and boundary conditions. Based on this theoretic framework we present the computation methods, provided by the computer algebra package *Varational Calculus*. The package is developed for the Maple8 [1] platform and divided in two modules – the *Variables* module and the *VariationalCalculus* module. The *Variables* module provides objects and methods concerning jet manifolds and is used by the *VariationalCalculus* module. The methods of the *VariationalCalculus* module allow us to determine the equations of motion and the corresponding boundary conditions for a given Lagrangian system. The application of this package to a Timoshenko beam shows, how one uses the proposed methods for engineering problems.

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Physiology and Medicine

SIMPLIFICATION OF A MATHEMATICAL MODEL FOR THE EXERCISE METABOLISM

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An important task within sports medicine is the diagnosis of the metabolic performance of individuals. For this purpose usually the response of the peripheral blood lactate concentration to exercise is studied, even though it does not allow a detailed reflection of the dynamics of the metabolic processes within muscles. Modelling and simulating can contribute to an increased understanding of system dynamics, both in qualitative and quantitative aspects.
Mathematical models of blood lactate kinetics have been developed to guide training or predict performance (e.g. [1] and [2]). To our knowledge no comprehensive model based on biochemical principles has yet been developed that quantitatively accounts for the dynamic behaviour and for the regulation of processes of the exercise metabolism in muscles.
In [3] we proposed such a model deduced by applying object–oriented modelling techniques. In brief, most simulation results show that the proposed model quite accurately reproduces dynamic effects observed in experiments and reported in literature. However, by now the discrepancy between the dimensionality of the model and the available data from measurements does not allow the identification of all model parameters in such a manner that all state variables are exactly predictable by simulation. These facts encourage a closer look at the mathematical model and the application of methods of control theory for an analysis of its main characteristics.
It is possible to show that the original aggregated mathematical overall model takes the form of a differential algebraic equation set (DAE). However, classical techniques of control theory for the analysis of system dynamics need sets of ordinary differential equations (ODEs). In order to apply these methods it is mandatory to simplify the DAE–description of the model to an ODE–description.
Starting from the model equations of the original work, the reasons for the algebraic constraints are determined. Algebraic constraints between descriptor variables result from model equations of fast reactions which are modelled under the assumption that the law of mass action holds for their substrates and products at all times. The module equations of such reactions are replaced by differential equations causing the same effect. The resulting overall model is a semi–explicit set of DAEs.
Further constraints result from reactions whose reaction rate is adapted to the rates of other reactions in such a manner that the concentration of a substrate or product remains constant at all times. After having deleted such metabolites from the mathematical model and after having performed necessary transformations the resuling mathematical overall model is given by a set of ODEs which has more state variables than differential equations.
Due to the stoichiometric properties of the metabolic system it is possible to classify the state variables in linearly independent and dependent state variables. Expressing the linearly dependent state variables by a linear combination of the linearly independent state variables leads to a simplified set of ODEs, for which the dynamic equilibrium can be calculated. From this functional dependencies between parameters and initial states are set up. Thereby the number of model parameters is reduced. Sensitivity analysis is applied to study the effect of parameters and initial conditions to rate their effects on the dynamic behaviour of the model for the exercise metabolism. The results give indications for further model simplifications and are exploited for an improved parameter identification.

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DEVELOPMENT OF A CEREBRAL AUTOREGULATION MODEL FOR USE WITH CLINICAL BLOOD FLOW MEASUREMENTS

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Autoregulation is the intrinsic ability of certain vessels in the brain to maintain cerebral blood flow (CBF) despite significant changes in arterial blood pressure (ABP). This important defence mechanism of the brain, the control of which is currently not well understood, is achieved through the constriction and dilation of small arteries and arterioles. It is important to understand how this mechanism operates in order to deal successfully with patients whose autoregulation has failed or is diminished. Although a large number of studies have been carried out, both in *vitro* and in *vivo*, there are clear limitations on experimental investigations. Successful studies of dynamic regulation have focused on the changes in CBF caused by changes in ABP: for example, transcranial dopplers (TCDs) may be used to measure maximum blood velocity in the major arteries supplying the brain, such as the middle cerebral artery (MCA) (see for example [1]). Although a number of mathematical models have been developed, most represent the autoregulatory mechanism in only an abstract form and concentrate instead on complex descriptions of cerebral anatomy (e.g. [3]). In addition to containing variables and parameters which may be impossible to measure and difficult to estimate, these models often do not distinguish between the possible causes of any deficiency in autoregulation.

A model of blood flow in the MCA has been developed [2], approximating the vessel as a rigid pipe (the limiting solution for elastic vessels attached to surrounding tissue mass [4]). The former provides a direct physiological interpretation of clinical measurements through a simple abstract description of the complete autoregulatory process. In this paper it is shown that fully developed blood flow in the MCA due to small amplitude changes in ABP may be approximated by a parabolic profile. In addition to replicating the results of [2], the model allows for considerable flexibility in modelling the autoregulatory response. The system has been extended to model the autoregulating vessels themselves, allowing for the inclusion of radius dependent mechanisms, in addition to those dependent on flow (or velocity) and pressure (or pressure gradient). Comparison with clinical results indicates the deleterious effect on response rate of strong dilation.

Much previous work has focused purely on flow rather than velocity, related through Ohm's law to pressure and vessel resistance. This is, however, based upon Poiseuille flow which is both parabolic and steady. The model presented here continues to assumes fully developed flow, which is a crude approximation of true blood flow dynamics but provides a useful description of an average vessel's response. The advantage of the simplified model is that it provides a dynamic description of the relationship between flow, pressure and radius, based upon their values and rates of change. In addition it can be extended to include more sophisticated descriptions of the autoregulatory mechanisms while continuing to measure clinically measurable variables. This approach will, in future, allow for the investigation of hypotheses concerning these mechanisms which might otherwise be obscured by more complex models of cerebral anatomy.

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ASYMPTOTIC OF SOLUTIONS OF SINGULAR SYSTEM DESCRIBING THE DEVELOPMENT OF EPIDEMIC

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Mathematical model for control of epidemic process is based on the scheme of cross infecting and on the mechanisms forming the ability of a pathogen to stimulate syndrome disease (virulence). The aim of the study is to investigate how the level of mass vaccination u_0 influences on the change of virulent value V in final phase of fore-epidemic period. The specificity of the main model is to determine the variability of pathogen. The controlled epidemic process is described by the system of differential equations (1) where N_1, N_2, N_3 are the numbers of susceptible to diseases, sick and immune people accordingly, V – virulence, u – intensity of mass vaccination, α, c, m – coefficients of self-regulation, β – value inverse to duration of disease, q – value inverse to duration of immunity, H is total quantity of persons involved in the epidemic process.

$$\begin{cases} N_1 = H - N_2 - N_3, \\ dN_2/dt = \alpha V N_1 N_2 - (\beta + \beta')N_2, \\ dN_3/dt = \beta N_2 - qN_3 + u, \qquad u = \begin{cases} 0, \text{ where } t < 0 \\ u_0, \text{ where } t \in [0,T] \\ 0, \text{ where } t > T \end{cases} \\ dV/dt = (c_0 + c_1 - mN_3)V, \end{cases} \tag{1}$$

$$t_0 = 0,\ N_2(0) > 0,\ N_3(0) \geq 0,\ 0 < V(0) << 1$$

Since this system has a big parameter H, we can reduce it to the system with small parameter at the highest derivative. We can investigate above mentioned dependence using the theory of singular perturbance with the help of simpler equations [1]. ($N_2=Hn_2$, $N_3=Hn_3$, $\beta'=H\beta_0'$,$u'=u_0'/H$).

$$\begin{aligned} \mu \dot{n}_2 &= \alpha V(1 - n_2 - n_3)n_2 - (\mu\beta + \beta_0')n_2, \\ \dot{n}_3 &= \beta n_2 - qn_3 + u', \qquad \mu = 1/H << 1, \\ \mu \dot{V} &= (\mu c_0 + c_1(1 - n_2 - n_3) - mn_3)V, \end{aligned} \tag{2}$$

If $\mu=0$ then we have the system of slow changes [2]. If $n_2=V=0$ then we have a fore-epidemic period $[0,T']$ where the mass vaccination was build.

Using [1] the solution (1) is found as the sum of the *regular* series and the *boundary series*

$$x = \bar{x}(t,\mu) + \Pi x(\tau,\mu), \qquad x = (n_2, n_3, V), \tag{3}$$

We can simplify the series basing on some peculiarity of development of epidemic [3]. If the beginning of epidemic is the beginning of visible increase of sick people N_2 then for the analysis of dependence $V(u_0)$ we can use the solutions of the system of quick changes in the boundary sublayer. The system of quick changes is a result of change of variable $\tau=Ht$ in (2) with the initial data $t_0=T'$, $t\in[T',T]$. Finding the solutions of simplified system as power series of μ, we can build the equations for finding $n_2^0(t)$, $n_3^0(t)$, $V^0(t)$:

$$\begin{aligned} \dot{n}_2^{\,0} &= \alpha V^0(1 - n_2^{\,0} - n_3^{\,0})n_2^{\,0} - \beta_0' n_2^{\,0}, \\ \dot{n}_3^{\,0} &= 0, \\ \dot{V}^0 &= (c_1(1 - n_2^{\,0} - n_3^{\,0}) - mn_3^{\,0})V^0, \end{aligned} \tag{4}$$

with the initial data $n_3^{\,0}{}_{нач} = n_3(T')$, where $n_3(t) = \bar{n}_3 + (n_{3\,нач} - \bar{n}_3)\exp(-qt)$, $\bar{n}_3 = u'/q$. Having constructed the solutions of system (4) we can find the dependence between V^0 and u_0'. The qualitative analysis of the system for finding zero members of asymptotic expansion (4) gives necessary information about regarding the dependence between zero members of expansion and the level of mass vaccination.

The fundamental possibility of applying the theory of singular perturbance to analysis of behavior of special equations describing the development of epidemic was studied in this work. There was shown the possibility of getting the result with the help of simpler method, when boundary layer was broken into two sublayers.

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Set-Membership Modelling of Uncertainties in Dynamical Systems

OPTIMIZATION OF ECONOMIC GROWTH VIA OPTIMAL INVESTMENT IN R&D

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An endogenous growth model linking a smaller follower country to a larger autarkic leader through "absorptive capacities" enabling it to tap into the knowledge generated in the leading country was introduced by Hutschenreiter, Kaniovski and Kryazhimskii in [1]. It is built along the lines of the basic endogenous growth model due to Grossman and Helpman [2] with horizontal product differentiation, where technical progress is represented by an expanding variety of products. Based on a comprehensive analysis of the dynamic behaviour of the leader-follower model, a particular class of asymptotics was singled out. Any trajectory characterised by this asymptotics was shown to be a perfect-foresight equilibrium trajectory analogous to the one found for the basic Grossman - Helpman model. The evolution of the economy represented by this model is the result of decentralised maximising behaviour of economic agents. A perfect-foresight equilibrium trajectory generated by the model can therefore be referred to as "decentralised" or "market" solution. However, a market solution is not necessarily an optimal solution. The present paper is concerned with the model of optimal allocation of labour resouces to R&D introduced by Aseev, Hutschenreiter and Kryazhimskii [3], [4]. An important feature of this problem is that the goal functional is defined on an infinite time interval. In problems with infinite time horizons the Pontryagin maximum principle [5], is, in general, less efficient than in problems with finite time horizons. In particular, for the case of infinite time horizons the natural transversality conditions may not be valid [6]. In paper [3], using an approximation approach to the investigation of optimal control problems with infinite time horizons [7], the existence of optimal control was proved and an appropriate version of the Pontryagin maximum principle was developed. Moreover, a particular case when the amount of labour allocated to R&D in the leading country exceeds the total labour force in the follower country was investigated. In the present paper, we give sketches of proofs of general results obtained in [3], and then we qualitatively analyse the solutions of the Hamiltonian system, arising through the implementation of the maximum principle in the case when the elasticity of substitution between any two products is equal to 2 while the other parameters of the model can take all possible values. Namely, we find that in this case the global optimizers are characterised by specific qualitative behavior; this allows us to select the unique optimal regime in the pool of all local extremals.

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PROPERTIES OF OPTIMAL ELLIPSOIDS APPROXIMATING REACHABLE SETS OF UNCERTAIN SYSTEMS

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The ellipsoidal estimation of reachable sets is an efficient technique for the set-membership modelling of uncertain dynamical systems [1–4]. Denote by $E(a, Q)$ the n-dimensional ellipsoid given by

$$E(a, Q) = \{x : \big(Q^{-1}(x - a), (x - a)\big) \leq 1\}, \tag{1}$$

where $a \in R^n$ is its center and Q is a positive definite $n \times n$ matrix. Consider a linear dynamic system

$$\dot{x} = A(t)x + B(t)u + f(t), \quad t \geq s, \tag{2}$$

where $x \in R^n$ is the state, and $u \in R^m$ is an unknown perturbation bounded by the ellipsoid $u(t) \in E(0, G(t))$. The initial state belongs to the ellipsoid $x(s) \in M = E(a_0, Q_0)$. The *reachable set* $D(t, s, M)$ of system (2) is a set of all ends $x(t)$ of trajectories $x(\cdot)$ of the system under the imposed constraints and conditions. We study optimal outer ellipsoidal bounds on reachable sets: $E(a(t), Q(t)) \supset D(t, s, M)$. Various optimality criteria are considered, the main attention being paid to the criterion $J = (Qv, v)$ related to the projection of an ellipsoid onto a given direction. Here, $v(t)$ is a given n-vector function. Differential equations for both locally and globally optimal outer approximating ellipsoids are derived and analyzed. For locally optimal ellipsoids, the time derivative dJ/dt is minimal, whereas for globally optimal ones, the criterion $(Q(T)v_T, v_T)$, where T is a given time instant, is to be minimized. The center and the matrix of both locally and globally optimal ellipsoids satisfy the following equations

$$\dot{a} = A(t)a + f(t), \quad a(s) = a_0, \tag{3}$$

$$\dot{Q} = AQ + QA^T + hQ + h^{-1}K, \quad K(t) = B(t)G(t)B^T(t), \quad Q(s) = Q_0.$$

For locally optimal ellipsoids, $h = [(Kv, v)/(Qv, v)]^{1/2}$. For globally optimal ellipsoids, $h = [(K\psi, \psi)/(Q\psi, \psi)]^{1/2}$, where $\psi(t)$ satisfies the adjoint equation and initial condition

$$\dot{\psi} = -A^T(t)\psi, \quad \psi(s) = v_T. \tag{4}$$

Locally and globally optimal ellipsoids coincide, if $v(t) = \psi(t)$, where $\psi(t)$ satisfies (4). These ellipsoids touch reachable sets at all instants $t \in [s, T]$. The equations of approximating ellipsoids for the criterion J are simpler than for other criteria. By means of special changes of variables, nonlinear equations (3) for Q are simplified and reduced to the forms, where either $A = 0$ or $K = I$. Here, I is the unit matrix. Asymptotic behavior of ellipsoids is analyzed in two limiting cases. If the initial set is a point $x(s) = a_0$, then $Q(s) = 0$, and equation (3) for Q has a singularity at $t = s$. The expansion of the solution $Q(t)$ for small $t - s$ is obtained. This expansion can be used for starting the numerical integration of equation (3). Also, asymptotic behavior of $Q(t)$ at infinity (as $t \to \infty$) is analyzed.

A special control problem for a system subjected to uncertain perturbations is investigated in the framework of optimal ellipsoidal estimation of reachable sets. The obtained results are applicable to various problems of state estimation and control in the presence of uncertain perturbations and observation errors.

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SET-VALUED SOLUTIONS TO IMPULSIVE DIFFERENTIAL INCLUSIONS

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The paper deals with the state estimation problem for impulsive control system described by differential inclusions with measures. The problem is studied under uncertainty conditions with set–membership description of uncertain variables which are taken to be unknown but bounded with given bounds.
Such problems arise from mathematical models of dynamical and physical systems for which we have an incomplete description of their generalized coordinates (e.g., the model may contain unpredictable errors without their statistical description). In this setting instead of an isolated trajectory of the dynamical control system we have a tube of such trajectories and a phase state vector should be replaced by a set of its possible values. The techniques of construction the trajectory tubes and their cross-sections that may be considered as set-valued state estimates to differential inclusions with impulses are studied.

We consider a dynamic control system modelled by a differential inclusion

$$dx \in \mathcal{F}(t,x)dt + B(t,x)dv(t), \quad x \in R^n, \tag{1}$$

with unknown but bounded initial condition

$$x(t_0) = x^0, \quad x^0 \in X^0, \tag{2}$$

and with certain control variables represented by vector measures $dv(t)$ (generalized or impulsive controls). In such problems the trajectories $x(t)$ are discontinuous and belong to a space of functions with bounded variation. Among problems related to treatment of dynamic systems of this type let us mention the results devoted to the precise definition of a solution and publications on optimal control problems.

In the estimation problems the so-called measurement equation is considered also

$$y(t) = g(t, x, \xi(t)) \tag{3}$$

with $\xi(t)$ being the unknown but bounded "noise" or disturbance. The latter equation may be expressed as the state ("viability") constraint.
One of the principal points of interest of the theory of control under uncertainty conditions is to study the set of all solutions $x[t]$ to (1)-(2). The "guaranteed" estimation problem consists in describing the set $X[t] = \cup\{x[t]\}$ that is actually the reachable set (the information domain) of the system at instant t. The set $X[t]$ may be treated as the unimprovable set-valued estimate of the unknown state $x(t)$ of the system. The paper is devoted to some approaches to the solution of this estimation problem.

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OPTIMAL AND SUBOPTIMAL ALGORITHMS IN SET MEMBERSHIP IDENTIFICATION

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We study optimality properties of identification algorithms in a set membership framework. We deal with restricted complexity (conditional) identification, where approximations (models) to a possibly complex system are selected from a low dimensional space. We discuss the worst- and average-case settings. In the worst-case setting, we present results on optimality, or suboptimality, of algorithms based on computing the unconditional or conditional Chebyshev centers of an uncertainty set. In the average-case setting, the optimal algorithm is defined by the projection of the unconditional Chebyshev center. We give explicit formulas for its average errors, which allow us to see the contribution of parameters of the identification problem to the minimal error.

REACHABILITY UNDER UNCERTAINTY AND MEASUREMENT ERRORS

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Abstract.

The problem of calculating sets reachable by a controlled system is one of the basic topics of modern Control Theory. It is motivated by many applied issues – from problems in navigation and traffic safety to verification of algorithms for complex transition systems.

A more complicated problem, though closer to reality, is the one of reachability under disturbances which describes the sets of points, whose neighbourhoods can be reached despite the unknown but bounded disturbances. A description of this problem for the case of linear systems was given in papers [1,2]. Here it is important to distinguish reachability under closed-loop (feedback) control from reachability under open-loop control.. The latter , in its turn, may be of the anticipative (maxmin) type or of the (nonanticipative) minmax type.

An intermediate reachability problem is when the control is selected as piece-wise open-loop, when one is allowed to change (correct) the open-loop control at isolated instants of time on the basis of available information which are the measurements of the state vector and also, in case of maxmin control, the values of the disturbance for the coming interval of time. In this sense the piece-wise open-loop control is also piecewise- feedback, with feedback signal arriving at prespecified points of correction.

The relations between all the mentioned types of reach sets decribed above are discussed in detail in paper [2]. The calculation of such sets through the techniques of "ellipsoidal calculus" is described in papers [3], [4].

The present paper discusses a situation which does not seem to be treated before, namely, when the information on the state space vector at points of correction arrives through partial measurements which are also corrupted by unknown but bounded noise. This situation requires combination of earlier methods of calculating reach sets with the techniques of guaranteed (set-membership) estimation theory [5]. For systems with linear structure and ellipsoidal or box-valued hard bounds on the unknown items the present report gives the solution scheme for the problem and indicates routes for effective calculation and computer animation.

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INTERVAL SOLUTIONS FOR INTERVAL ALGEBRAIC EQUATIONS

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In the framework of interval uncertainty, a well-known classical problem in numerical analysis is considered, namely, to find "the best" interval solution for interval system of linear algebraic equations. This problem is known to be NP-hard and can be solved via multiple linear programming [1,2]. In present paper, a simple approach is proposed for some particular models of interval uncertainty.

We consider a system of linear algebraic equations $(A+\Delta A)\,x = b+\Delta b$, where A and b are nominal real data while all components of system matrix or right-hand side vector are assumed to belong to equal intervals, i.e. $||\Delta A||_\infty \le \varepsilon$ and $||\Delta b||_\infty \le \delta$. The problem is then to find the interval solution $\mathbf{X}$ of linear interval system. In other words, we need to describe explicitly the so-called solution set X that is all possible system solutions x under given constraints and to derive its interval outer-bounding estimates $\mathbf{X} \supseteq X$.
The algorithm obtained gives an optimal interval solution without linear programming and exploit the results by Rohn [3] It is based on searching for 2^n vertices of the convex hull of the solution set. Each vertex can be found by solving a scalar equation. The method is tractable for moderate-size problems. For large-scale problems an effective overbounding technique is developed.

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APPLICATION OF ELLIPSOIDAL ESTIMATIONS TO SATELLITE CONTROL DESIGN FOR FORMATION FLYING IN THE PRESENCE OF UNCERTAINTIES

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The equations of relative motion of a small satellite with respect to another one, (moving along the prescribed trajectory), are presented (based on the results given in [1]). The corresponding equations for relative motion errors caused by the uncertainties in initial conditions and control implementation imperfections are linearized. The obtained linear equations are analyzed and the evolution equations for optimal ellipsoidal estimates of these errors are derived. The ellipsoidal bounding of reachable sets is an efficient approach for the modelling of uncertain linear dynamical systems (see, e.g. [2–5]).
The procedure constructed in the paper allows to take into account the results of discrete observations and design control aimed to compensate the disturbances between measurements performed with errors. These measurements are assumed to be performed with small errors. A numerical example is given . It shows illustrates the fact that the presented control design algorithm is quite efficient, and it allows to keep the error between the real and desired motion close to zero.

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STRUCTURED IDENTIFICATION OF COMPLEX NONLINEAR SYSTEMS

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In the paper the problem of identifying discrete time nonlinear systems in regression form from finite and noise-corrupted measurements is considered. According to the specifications about identification accuracy that may be needed, a good exploration of the regressor domain of interest have to be ensured by the experimental conditions. This problem becomes very significant for growing dimension of the regressor space, leading very easily to computational complexity problems and to inaccurate identified models. These difficulties are significantly reduced if, using information about the physical structure of the system to be identified, this can be decomposed in interacting subsystems. Using this structural information, the high-dimensional identification problem may be reduced to the identification of lower dimensional subsystems and to the estimation of their interactions. Typical cases considered in the literature are Hammerstein, Wiener and Lur'e systems, but the paper shows that the approach can be extended to more complex structures composed of many subsystems and with nonlinear dynamic blocks, using as example the identification of a half-car model for vehicles vertical dynamics, where nonlinear suspensions and tyres are considered. Assuming that the road profile is given and that front and rear vertical accelerations are measured, an experimental setup easily realizable in actual experiment on real cars, the half-car model is decomposed as a generalized Lur'e system, consisting of a linear MIMO system, connected in a feedback form with the two nonlinear dynamic systems through not measured signals. An iterative identification scheme is proposed, which makes use of a set membership method for the identification of the nonlinear dynamic blocks. This method does not require assumptions on the functional form of the involved nonlinearities, thus circumventing the identification accuracy problems that may be generated by considering approximate functional forms. The numerical results demonstrates the effectiveness of the the proposed approach.

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MODELLING AND ANALYSIS OF COMBINED ELECTRONIC AND MICRO - MECHANICAL SYSTEM

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Abstract. Modelling of micro-mechanical systems in combination with integrated electronic systems is a complex task demanding the knowledge of mechanical and microelectronic design in combination with system modelling expertise. It is becoming increasingly important due to the fast growth of the so called "smart sensors" applications based on micro-mechanical devices. Our task was to create a reliable model of micro-mechanical acceleration sensor to be used for further development of mechanical and electrical part of the system. The modelling inputs were the measurement data of the prototype devices comprising static characteristics of the device and system responses to step function excitation. Together with the known physical properties and basic theoretical equations these data enabled us to create the described model which showed a high level of compliance to measurement results.

Model-based estimation of contact forces in rotating machines

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Model-based fault detection in rotating machines has been the focus of several scientific and industrial efforts during the last decade. In practice the measurement of contact forces is difficult. The forces can only be obtained via the resulting vibration effects (displacement, strain). In this contribution, model-based observer techniques are used to estimate contact forces between rotor and housing of rotating machines.

Core of this contribution is the detailed introduction and combination of two model-based Proportional-Integral-Observer (PIO) approaches used to solve the contact force estimation task. The approaches use a minimal number of displacement measurements (using one or two sensors). Both observers are based on mathematical models of the elastic structure. An advantage of the PIO approach is that no model of the affecting disturbance is necessary. This allows the application to problems, where no model is available or the known model is not useful because of its complexity. An application to estimate unknown impact forces acting on a fixed elastic beam structure via PIO was published in (1).

The classical PIO design as used in (1) works with high gains. External disturbances affecting an elastic structure can then be estimated. But the conventional design is not particularly suitable for handling measurement noise, because the noise is amplified by the high gains. For state estimation in (3) a PIO design, which permits to attenuate measurement noise, is proposed. A reformulation of the observer design is given in such a way that the measurement noise is not affected by the observer gain. In this paper the classical PIO design as used in (1) is extended by the reformulation that is given in (3). The new formulated PIO design achieves satisfying results (estimation of unknown inputs) while the measured signal is affected by measurement noise. Since measurement noise in practical applications cannot be completely suppressed, this is an important step to get better results with the PIO and to make the observer technique more suitable for practical applications.

A simulation example, dealing with a rotating shaft and acting contact forces on a blade, is carried out to analyze the two different PIO approaches. Further experimental results of contact force estimation between a blade and housing are presented (2).

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MECHANICAL AND ACTIVE CAR DIFFERENTIALS: DETAILED AND REDUCED DYNAMIC MODELS

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Recent automotive applications try to use active differentials in order to optimize the torque distribution on the wheels for traction maximization, driving comfort, stability and safety of the vehicle.
The differential (see Fig.1) is a mechanical system necessary to allow different rotation speeds of the wheels during a cornering track, ensuring a uniform transfer of the traction forces on the road. To avoid wheels spinning in some critical conditions (like on iced roads) it is necessary to lock the conventional differential. This can be done in different ways: the mechanical limited slip differential uses friction plates and cones activated by the secondary torque; the active limited slip differential is based on an electro-hydraulic control for locking the differential in a wide range of operating conditions; a novel mechanical scheme, the evolved active differential, uses multiple actuators to better control the torque transferred at the wheels. In the paper, detailed and reduced dynamic models of these four different types of differential are presented by using the Power-Oriented Graphs (POG) modeling technique.

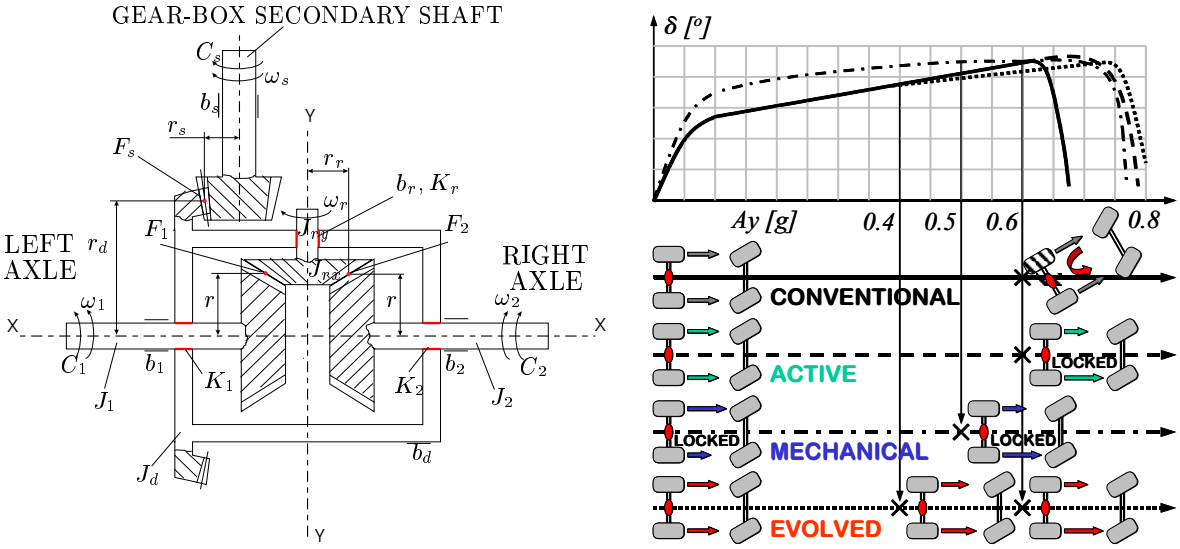

Figure 1: Simplified mechanical scheme of a conventional car differential (left) and steering pads (right).

The steering pads of a rear traction car running a left corner of constant radius (10 m) at a constant longitudinal acceleration ($A_x = 0.3$ g) with the four kinds of differentials are shown on the right of Fig.1, where δ is the steering wheel angle. This graph shows the effects of the differentials. The solid line represents the typical understeering behaviour of a car equipped with a conventional differential: as soon as the lateral acceleration A_y becomes greater than 0.6 g, due to the dynamic lateral load transfer, the rear left wheel starts spinning and the vehicle becomes uncontrollable. The active differential (dashed) starts working in this situation, when the inner wheel would rotate faster than the outer one, it locks the two wheels so that more torque is transferred to the external (right) wheel, consequently the car is controllable until the car physical limit close to 0.8 g. The mechanical limited slip differential (dash-dotted) has a similar behaviour, but it shows an unpleasant understeering at low lateral accelerations because, due to the longitudinal acceleration, the differential is already locked and more torque is transferred to the inner wheel. The mechanical and the active limited differentials can only transfer torque from the faster to the slower wheel, the evolved differential (dotted) overcome this limit and can manage the torque repartition for a wider range of lateral accelerations improving the guidability.

Two-sided Arnoldi Algorithm and Its Application in Order Reduction of MEMS

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Direct dynamic simulation based on fully meshed structures of a Micro Electro Mechanical System (MEMS) is computationally intensive, making it difficult to use in system level simulators. In order to perform rapid design prediction and optimization, it is essential to build accurate and easy to use reduced order dynamical models for these devices. For the reduction of high order systems, Krylov subspace methods are probably the best choice today, see e.g. [1, 2]. They define a projection from the high dimensional space of the original model to a lower dimensional space and vice versa and thereby define the reduced order model. Some of the characteristic parameters of the original model and the reduced model - the so-called *moments* - equal each others, which is also referred to as *moments matching*.
The n-th order single-input-single-output system to be reduced is defined in the general state-space representation

$$\begin{cases} \mathbf{E}\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{b}u(t), \\ y(t) = \mathbf{c}^T\mathbf{x}(t). \end{cases} \tag{1}$$

By applying the projection $\mathbf{x} = \mathbf{V}\mathbf{x}_r$ where $\mathbf{V} \in \mathbb{R}^{n\times q}$ and $q < n$, to system (1) and then multiplying the state equation by transpose of some matrices $\mathbf{W} \in \mathbb{R}^{n\times q}$, a model with reduced order q can be found,

$$\begin{cases} \mathbf{W}^T\mathbf{E}\mathbf{V}\dot{\mathbf{x}_r}(t) = \mathbf{W}^T\mathbf{A}\mathbf{V}\mathbf{x}_r(t) + \mathbf{W}^T\mathbf{b}u(t), \\ y = \mathbf{c}^T\mathbf{V}\mathbf{x}_r(t). \end{cases} \tag{2}$$

It can be proved that, if $\mathbf{V}$ and $\mathbf{W}$ are bases of the input and output Krylov subspaces, respectively then, the first $2q$ moments match (two-sided method) and the transfer function of the reduced order models is independent of the particular choice of the bases [3].
Thus, finding a basis for a given Krylov subspace is necessary to calculate a reduced order model. Computing such a basis for a large scale system involves numerical problems and there exist some algorithms to avoid numerical errors. In two-sided methods, Lanczos algorithm [2] is commonly used which finds a bi-orthogonal basis for input and output Krylov subspaces. In this paper, we introduce a new method called two-sided Arnoldi to find the bases necessary for projection and calculating the reduced order model. This new method in comparison to Lanczos is *numerically stable and easier to implement* while performing the same reduced order system. This method uses Arnoldi algorithm twice, once for the input Krylov subspace to find the matrix $\mathbf{V}$ and then for the output Krylov subspace to find the matrix $\mathbf{W}$. In this way, each basis is orthogonal instead of bi-orthogonality in Lanczos algorithm.
A stopping criterion has also been presented that can be used to find a suitable order for a reduced model. This measure is calculated in each iteration and there is no need to break the loop. In addition, a remark to avoid computation of inverse of a large matrix is proposed which leads to a faster algorithm.
In particular, we apply this method to a class of high energy MEMS actuators which integrates solid fuel with three silicon micromachined wafers [1]. The governing equations results in a linear system of 1071 ordinary differential equations. By comparing the results with the commonly used Arnoldi algorithm, we found that the error in two-sided method is much less and it is possible to find reduced order models of lower order with approximately the same error as the one-sided method.

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EFFECTIVE ELASTIC COEFFICIENTS IN AN INITIALLY STRESSED GRAVITATING BODY AND A MATHEMATICAL MODEL FOR PREDICTION OF LIQUID CORE INSIDE A PLANET.

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ABSTRACT

Due to variation of temperature, slow process of creep, gravitational pull, weight of overburden layer etc a huge quantity of stresses, called initial stresses, are stored inside a planet. These stresses would change the elastic coefficients of the planet and should have effect in propagation, reflection and refraction of seismic waves. For more accurate seismic studies it is of interest to study the behaviour of elastic coefficients under initial of stresses.

The paper studies the effect of the initial stresses as well as gravity field on the elastic coefficients and expressions of Effective Elastic Coefficients are obtained at any depth.

The result has been extended to predict the liquid core inside the planet and shows that the earth has liquid core at the depth 3000 km approx, the Moon has no liquid core where as the Jupiter has a big liquid-dome.

The paper also refutes the solid inner core of the earth .

SIMULATION OF DISCONTINUOUS DYNAMIC PROPERTIES IN CONSTRAINED MECHANICAL SYSTEM WITH FRICTION AND VARYING CONTACT

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The discontinuities phenomena/effects has presence in multibody dynamics when sliding friction contact and clearance are introduced to the moving machine parts. The clearance has usually manufacturing or constructive nature and provides the relative mobility of their joint parts. For some high-speed kinematics pairs mentioned above real physical attributes as multiple and friction contact have direct influence on generating value of constraint reaction forces and corresponding force transfer functions (FTFs) for each contact-cases of colliding bodies. The value of FTFs are establish the load capacity and energy losses of contact pair, that depending on the dynamical environment. The discontinuity parameter associated with the set of FTFs and formulated in the term of Discontinuity Kernel (DK). Every components (FTFs) of DK defines the structure-variant topology and different systems states (ST=var) on the force level. The mathematical fundamentals and relevant terminology of the theory of systems with discontinuity structure are well developed and presented in [1]

Many researchers have studied the effect of active contact forces in connected machine parts, which modeled as applied and constraint forces. A large variety of contact configurations with rigid body approach and with different industrial applications have been considered by F.Pfeiffer, Ch.Glocker, D.Baraff, T.Klisch and many others scientists [2,3,4,5,6]. The mathematical description of such constrained mechanical systems may be in general expressed in the form of nonlinear differential–algebraic equations (DAEs) or in residual form by ordinary differential equations (ODEs) with Discontinuities in the right hand side. The numerical treatment of the discontinuous system presented by E.Eich-Soellner and C.Fuhrer in [7]. The solution methods include special numerical routines that based on control–oriented approach with switching conditions for modeling the transitions between closed contact-cases in multibody dynamics.

In this paper we consider Two-Sided Wedge Mechanism (TSWM) as constrained Multibody Rigid System with holonomic, time dependent constraint including sliding friction and varying contact (via existing clearance) on inclination active/closed surfaces of wedge segments. The TSWM is a Design Inertial Dynamic Model of a separate class of Mechanical systems with Worm gearing that have wide applications in machine industry. The meshing action and contact-cases in the Worm Kinematic Pair is quite similar to that of TSWM due to the worm that is of screw thread configuration.

The main idea of this paper is to discuss the new technique for generating the equations of motion and constraints equations that satisfying all conditions on friction and varying contact-for proposed model TSWM and elaboration the control-oriented (switching) algorithms for numerical simulation. The results have been computed by MATLAB ODE tools and demonstrate some advantages of proposed formulation of mathematical and dynamic model with varying structure properties. We can also obtain by simulation tools more details information about influence of inertial, force and contact sliding configuration on dynamic load capacity and internal energy losses in the Worm Drive Mechanical Systems under consideration.

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Process Engineering and Process Simulation

HYSDEL MODELING AND SIMULATION OF HYBRID DYNAMICAL SYSTEMS

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This paper presents the modeling framework for hybrid dynamical systems, where the system is modeled as *discrete hybrid automaton* (DHA) using high level modeling language HYSDEL (HYbrid System DEscription Language). Such a model can be later translated into *Mixed Integer Dynamical* (MLD) modeling framework [2]. Three different approaches to simulate MLD system are discussed and the efficiency is compared. First approach is the usage of the *mixed integer linear programs* (MILP). This approach has certain disadvantages, therefore two special simulation algorithms, which overcome these problems was developed.

Hybrid systems are the combination of logic, finite state machines, linear discrete-time dynamic systems and constraints. The interaction between continuous and discrete/logic dynamic can be connected through *A/D* (analog to digital) and D/*A* interfaces. According to [3] such a system can be modeled as *discrete hybrid automaton* (DHA). DHA model of a hybrid system is described by modeling language called *HYbrid System DEscription Language* (HYSDEL), which represents an abstract modeling step [3]. The associated HYSDEL compiler translates the DHA model into an equivalent MLD form (1).

$$\begin{aligned} \mathbf{x}(k+1) &= \mathbf{A}\mathbf{x}(k) + \mathbf{B}_1\mathbf{u}(k) + \mathbf{B}_2\boldsymbol{\delta}(k) + \mathbf{B}_3\mathbf{z}(k) \\ \mathbf{y}(k) &= \mathbf{C}\mathbf{x}(k) + \mathbf{D}_1\mathbf{u}(k) + \mathbf{D}_2\boldsymbol{\delta}(k) + \mathbf{D}_3\mathbf{z}(k) \\ \mathbf{E}_2\boldsymbol{\delta}(k) + \mathbf{E}_3\mathbf{z}(k) &\le \mathbf{E}_1\mathbf{u}(k) + \mathbf{E}_4\mathbf{x}(k) + \mathbf{E}_5 \end{aligned} \tag{1}$$

Using the current state $\mathbf{x}(k)$ and input $\mathbf{u}(k)$, the time evolution of (1) is determined by solving $\boldsymbol{\delta}(k)$ and $\mathbf{z}(k)$ from inequalities in (1), and then updating $\mathbf{x}(k+1)$ and $\mathbf{y}(k)$ from equalities in (1). The MLD system (1) is assumed to be completely well-posed, i.e. for a given state $\mathbf{x}(k)$ and input $\mathbf{u}(k)$ the inequalities in (1) have a unique solution for $\boldsymbol{\delta}(k)$ and $\mathbf{z}(k)$. Obtaining the values of the auxiliary variables $\boldsymbol{\delta}(k)$ and $\mathbf{z}(k)$ presents a bottleneck in a simulation of a hybrid system modeled as MLD. The variables $\boldsymbol{\delta}(k)$ and $\mathbf{z}(k)$ can be computed by defining and solving the *mixed integer linear problem* (MILP) Because the system is *well posed* the solution is unique and only one solution to the system of inequalities exists. The disadvantage of the presented approach is the usage of the mixed integer optimization algorithms, which can be time consuming or even not able to find a feasible solution. To overcome these problems two special algorithms were developed, which are based on the knowledge of transformation DHA into MLD and are able to compute a values of $\boldsymbol{\delta}(k)$ and $\mathbf{z}(k)$ "explicitly", i.e. without iterations. Such approach is of course much faster. First algorithm is based on direct $\mathbf{E}_1,...,\mathbf{E}_5$ matrix manipulation, while the second one is a part of a recently released HYSDEL version 2.0.5. The both approaches are taking into account the MLD model building procedure.

The presented modeling approach and associated simulation algorithms are used to simulate a production of a *multi product batch plant* [1]. The multi product batch plant is modeled as DHA and transformed into equivalent MLD representation. The system is simulated first with the use of MILP optimization algorithms and then with the use of special designed algorithms. The results show that the use of the latter is much faster and more robust compared to the use of MILP optimization algorithms.

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Dynamic Model of a Rotary Kiln for Process Simulation and Control

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Many metallurgical processes include heterogeneous reactions, where the reacting species are captured in different physical phases. Typically a loose solid phase is contacted by a gas-flow in a rotary-kiln or multiple-hearth-furnace. A mathematical model of such a thermo-chemical system was developed to describe mass-flow and temperature of gas and bulk and the concentration of the main species.

For this process a multiple-hearth-furnace is used (see Figure 1), where the bulk-media is fed at the top of the furnace while the gas as a heating media and reactive partner enters from different inlets in counterflow to the bulk. Transportation of the bulk-media is carried out by a rotating shaft with bladed arms so that the media is transported from outside to inside in one stage and back in the following stage, and so on.
To derive a simple model of the process several assumptions were made: Every stage is considered to be ideally stirred and therefore consists of a homogenous gas- and bulk-layer. Although the reaction is known to be heterogenous, a simple homogenous rate-law is used, summing up every single effect concerning the reaction in a global rate-law. Furthermore, some of the material-constants (e.g. heat capacities, heat conductivity) are assumed to remain constant. Mathematical modelling of the multiple-hearth-furnace was done by setting up the balance-equations for every stage and using the experimentally derived rate-laws for the source- and drain-terms.

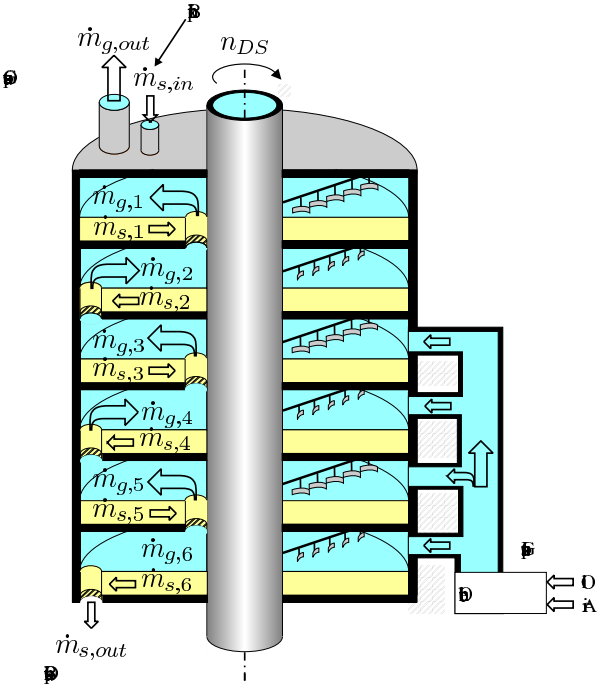

Figure 1: Scheme of a Multiple Hearth Furnace

To validate the dynamic model of the roasting-process various experiments were carried out on the original plant. From these results validation showed excellent consistency of the model-transport-behaviour and the thermodynamic model. Especially the bulk temperature at the set-point can be predicted accurately and the temperature-gradient for a changing set-point shows a very good match with measurement data. The correct simulation of the bulk-temperature is very important for control purposes on the real plant, as the temperature has a strong influence on the reaction-rate.
Validation of the chemical model showed unsatisfying accuracy and therefore the current reaction-rate-law has to be adjusted.

The dynamic model of the multiple-hearth-furnace has been successfully used for simulation and controller design, especially the thermodynamic part. The very simple chemical reaction-rate-law used is insufficient and has to be replaced. Therefore further work is now in progress including a systematic series of reaction experiments to establish a better reaction-rate-law.

MODELLING AND SIMULATION OF AN INDUSTRIAL ACTUATOR VALVE FOR FAULT DIAGNOSIS BENCHMARK

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Faults are usually the main cause of loss of productivity in the process industry. One of the most important type of equipment present in process industry is the actuator valve. A fault in an actuator valve may lead to a halt in production for long periods of time, but also may have security implications. If a fault is detected in its early stages a quick intervention can often prevent serious consequences to the ongoing process. Therefore, there is a need for fault diagnosis systems (FDI) that detect and isolate a fault as soon as it occurs. The design and performance testing of FDI systems for industrial processes often requires a good and efficient simulation model since the actual system is not available to generate the large amount of normal and faulty operational data needed for design and testing.
This paper addresses some fundamental modelling and simulation issues for a benchmark definition in the field of fault diagnosis in process industry. In particular, an industrial actuator valve for flow control will be extensively modelled considering the most relevant underlying physical phenomena and all auxiliary hardware inherent to these industrial devices. Normal operation conditions as well as faulty conditions are considered at the modelling and simulation stages, which results in a valuable industrial benchmark problem to assess the performance and reliability of fault diagnosis systems to be applied in process industry. Several of the most important faults, single and multiple, abrupt and incipient faults are modelled and implemented in the simulator. The numerical stiffness of the overall model is analysed. Several simulation results for normal and faulty operation conditions are presented and validated in relation to the actual real operating conditions in a process industry, as shown in the Figures below.

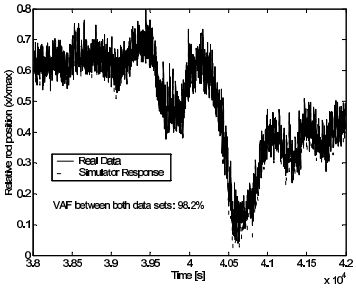

Figure 6 – Validation of real and simulation data for the rod's position in normal operation.

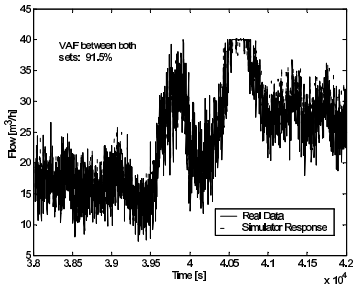

Figure 7 – Validation of real and simulated data for the flow in normal operation.

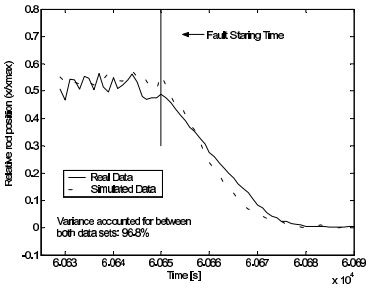

Figure 8 - Validation of real and simulation data for the rod's position for fault f14.

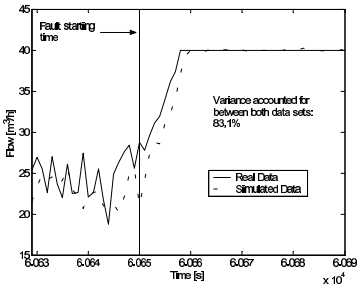

Figure 9 - Validation of real and simulation data for the flow for fault f14.

DISCRETE MODELLING OF CONTINUOUS GRINDING MILL-CLASSIFIER SYSTEMS

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A discrete mathematical model and computer program has been developed for analysis and design of the continuous grinding mill-classifier systems. In the model, the mixing of the material to be ground by the axial dispersion model, the breakage kinetics by the first order breakage law, and the classifier by a general classification function are described. The computer programs were developed using language C and MATLAB. The mathematical model and computer programs are suitable for simulation based analysis and design of mill-classifier systems.
This model may suggest an idea for deriving another mathematical models, which origin from different industrial, scientific or economic areas.
Considerable properties of the model are: non-negativity, conservation of the mass, stability.

In a number of grinding systems, mixing and breakage of particles occur simultaneously, so that mixing of the material to be ground may affect the efficiency and productivity of the system significantly. The influence of mixing was studied in a number of works [1-3], but the effects of mixing and the classification has been studied only recently [4]. The aim of this paper is to present the details of a discrete model, describing the mill-classifier systems under general operational conditions, and to analyze the properties and the behavior of the model by simulation.

The discrete mathematical model of the mill-classifier system can be given in the form of a set of recursive linear equations [4]. Often, the matrix form of the discrete model is rather suitable to study the behavior of the system. The paper shows deriving the matrix form of the model taking into account the recycling and delay. The form of the model is as follows:

$$\underline{y}_{n+1} = \hat{C}\,\underline{y}_n + \hat{\underline{b}}_n,$$

where $\underline{y}_n = \begin{bmatrix} \underline{V}_{n-d} \\ \underline{V}_{n-d+1} \\ \vdots \\ \underline{V}_{n-1} \\ \underline{V}_n \end{bmatrix}$, $\hat{\underline{b}}_n = \begin{bmatrix} \underline{0} \\ \vdots \\ \underline{0} \\ P \cdot \underline{c} \end{bmatrix}$, $\hat{C} = \begin{bmatrix} O & E & O & \cdots & O \\ O & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & O \\ O & \cdots & O & O & E \\ \hat{R} & O & \cdots & O & T \end{bmatrix}$, $\underline{c} = \begin{bmatrix} c \\ \vdots \\ c \end{bmatrix}$,

Different types of closed circuit operation modes of the mill are involved and described.
From practical point of view, the system achieves the stationary state when the transients of the state variables become almost damped. In some cases of operation, however, stationary state does not exist inside the feasible region of operation, and the process approaches to the boundary of the feasible region of operation. This situation leads to the overloading of the mill, which is a heavy breakdown. The existence or non-existence of stationary states in the feasible region of operation is examined by evaluating the eigenvalues of the system matrices using the form of the model given above. The properties of the model are analyzed by evaluating the results of numerical experiments.

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A COLD ROLLING MILL MODEL FOR UNWINDING DIAGNOSIS

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The full-version of this publication deals with the modelling of single stand rolling mills, as found in the steel and metal industry. More precisely the focus lies on the *unwinding process*, which handles the unwrapping of the metal strip. The model is seeked in order to study the *diagnosability* of such systems, *i.e.* the possibility to detect the presence of faults using model-based diagnostic methods.

Process diagnosis and fault detection are increasingly important and necessary features of modern industrial equipment with always tighter quality requirements. Many analysis tools have been developed, such as signal trend analysis or preventive maintenance, to guarantee a maximised use of a plant. However these methods are limited to the detection of major failures and might succeed at a very late stage only. In opposition, model-based diagnostic methods have drawn attention in recent years since they allow to detect faults that might only affect the system in a subtile way, *e.g.* influencing the system's dynamics solely. Hence the early detection of major problems is possible. These methods, which use a model of the process for the supervision task, contain a lot of information about the expected behaviour of the plant, therefore the result of the diagnosis can be more precise.
As seen in Figure 1, since the model of the process lies at the chore of the diagnosis, it is crucial to derive a model which is both simple enough to allow a diagnosis with reasonable computing power and complete enough to realistically represent the system's behaviour.

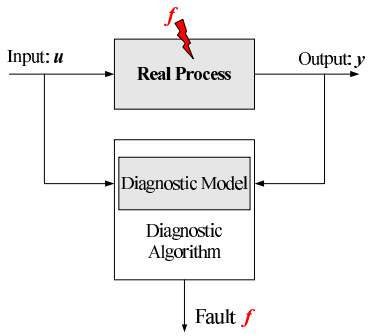

Figure 1: Fundamental concept of model-based process supervision

The paper presents two models of the considered unwinding process. First a *process model* of the unwinding is derived in Section 2. This model is a very thorough representation of the real process and takes many nonlinearities into account. In Section 3, this model is extended to allow the simulation of fault cases. Since it is difficult to obtain process measurements of faulty situations, this enhancement of the original model is necessary in order to test the diagnosis. This model has been implemented in DYMOLA for simulation.

A simplification of the process model using assumptions specific to rolling mills is then presented in Section 4. The obtained *diagnostic model* is linear and facilitates the implementation of standard diagnostic functions. Finally, results in simulation illustrate the successful use of the described models to detect faults at the uncoiler.

Software building for simulation of continuous casting of steel slabs and billets

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Information is provided about building mathematical model of continuous casting of steel slabs and billets including computer capacities aspects. The starting–point for discussion about this subject is solving of the partial differential equation of heat conduction for different boundary conditions by finite difference method. A numerical solution technique is implemented via *Pascal* and *C* computer programs running under Linux operating system and their speed of computation is compared. The accuracy of solution is tested by obtaining approximate solutions with two different sets of mesh points, one with the spacing of the other halved, and the temperatures at four representative spatial positions are compared.
The application software demands permanent services firstly in view of new process findings secondly in view of improvements in operating systems and program languages. Some years ago we developed a simulation model for continuous casting of steel slabs in order to attain initial temperature field in slabs charged hot into the pusher furnace. Although the governing equations were written in two dimensions the analysis was actually one dimensional due to lack of computer capacities. With the advent of Linux operating system for personal computers and possible program languages that run under this system an opportunity arose to upgrade the simulation model. One of the particular modeling objective, which is of practical industrial significance, is theoretical prediction of solidification front during continuous casting. The shell that is formed during continuous casting must be sufficiently thick to permit continuous withdrawal of the strand and withstand against ferro-static pressure of the remaining molten metal. The main prerequisite for accurate predictions is suitable grid and time resolution. A very fine mesh and small time steps are needed. Half-mm square elements and time increments of some thousandths of a second can be taken to be the problem solved accurately in a reasonably short time. In the model a wide range of operational parameters, such as steel grade, superheats, casting speed, cross-section, mould water temperature, water flow-rate and distribution as well as the heat transfer in the spray cooling zone were taken into consideration. In the continuous casting process molten metal flows from tun-dish into the water-cooled mold. Due to cooling a solid shell originates at the contact with mold walls. The steel strand consisted of a liquid pool and a solid shell is extracted bellow the mold into the compartment with water sprays at the speed that matches the casting speed. The solidification continues until the strand core becomes completely solid. Coming out of sprays the strand cools in the open-air mainly by radiation into the surroundings. The strand is cut with mechanical shears into slabs that are piled up under the hood, where the temperature in the slabs is equalized.
The heat conduction along the longitudinal axis of the strand can be ignored.[1] Consequently, the heat conduction equation for the transverse slice is solved by finite–difference method in two dimensions as if the slice were moving through regions of different boundary conditions at casting speed u covering a path $u.\Delta t$ in each time interval Δt. Heat conduction equation has to be solved for boundary conditions in the mold and spray chamber, for heat radiation into the surroundings and for temperature equalization in the slabs that are piled up under the hood. The results of calculation are temperature and solid shell profiles in the width and thickness direction along the casting machine as functions of time and operating parameters. In order to study the effects of the time step size on the convergence criterion, test trials were carried out. The stability study of solution according to the second law of thermodynamics shows that the stability criterion obtained from numerical equations approaches closely to the required value. The calculation of cooling history can be carried out with sufficient accuracy also in real time. Under the Linux environment, the use of *C* programming language with appropriate compiler options can speed up computations as compared to *Free Pascal compiler* by roughly assessing fourteen times.

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Chemical Process Engineering

AN OPTIMAL DESIGN OF HIGH DISPERSIVE REACTORS

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Many chemical reactors involve two distinct phases. In an automobile catalytic convertor, for example, the pollutant reactants are carried by the gaseous exhaust whereas the reaction is actually taken place on the solid ceramic *monolith*. In a packed bed reactor, being cooled by an external heat exchanger, the reactant within the reactor is often gaseous whereas the cooling jacket is a liquid. It is known that in such systems thermal destabilization often occurs which is due to an accumulation of heat released by the chemical/nuclear reactions within very legalized regions, known as hot-spots. Such a hot spot can sinter the catalyst, causing a run-away reaction [1], [2], and many more undesirable effects. It is hence important to design two-phase reactors with maximum heat dispersion capabilities.
It is known empirically that in a long conduit, variation in the heat convection velocity of each phase can actually produce significant thermal dispersion with an effective diffusivity orders of magnitude higher than the thermal diffusivity of each phase. However estimation of this convection-enhanced effective dispersion, known as Taylor dispersion, involves tedious moment or averaging analysis leading to difficulty in derivation of this effective dispersion.
In this paper, we consider a system in a tube shell configuration having two different phases, where the outer layer is solid while the inner part is fluid (liquid or gas). For this two-phase reactor, an *averaged* equation for the fluid temperature in the inner cylinder together with its effective dispersion coefficient is derived. This coefficient is in the form of an infinite series. Instead of a direct method to compute this coefficient, a compact method will be used.
It is shown that the effective thermal dispersion coefficient α_{eff} depends on a parameter β, the ratio of heat convection velocities of the solid phase and liquid phase, as well as on a parameter γ that represents either the interphase heat transfer (when the geometry is fixed) or the quotient of the shell thickness and the inner radius, $\delta = \Delta r/a$. For some ranges of the values β there is no local optimum value of α_{eff} with respect to γ. Outside these ranges, α_{eff} achieves its local optimal value at a unique γ. Hence an optimal high dispersive reactor can be obtained by optimising either the geometry or the type of material represented by the parameter γ.
In the case that the convective velocity for the solid phase is zero, the system is an approximate system for an automobile catalytic convertor. It has been shown in [3] that although the actual geometry of an automobile catalytic convertor is quite complex, an approximation using a cylindrical channel is very robust. For this case, in [3] an expression in the form of a series for the effective dispersion coefficient has been derived, and, after tedious algebra, a closed-form limit of this series. A comparison will show that the method presented here produces exactly the same result as in [3]. It is further shown that, for a given type of material, the expression α_{eff} depends only on δ. If δ_m is the optimal value for α_{eff} then this value is only sensitive for changes in $\hat{\alpha} = \alpha_s/\alpha_g$, when the quotient $\Lambda = (\rho c_p)_s/(\rho c_p)_g$ is small; when Λ is larger, the sensitivity is less. Here α, c_p and ρ are thermal diffusivity, heat capacity and mass density, respectively. The subscript s refers to the solid phase while subscript g refers to the fluid phase.

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MODEL OF A CONTINUOUS STIRRED TANK REACTOR USING BOND GRAPH FORMALISM

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The aim of this paper is to present an alternative approach to modelling in chemical engineering using port based modelling approach. One of the expected advantages of such an approach is the development of reusable models. Our approach is based on generalized bond-graph formalism as proposed by P. Breedveld [1]. It combines the axiomatic relation of the thermodynamics with pairs of conjugate variables (intensive and extensive) whose the product gives a power term. But secondly it is a graphical network language whose the model is composed of multi-port elements interconnected by a power continuous network. This paper is introductory and aims to provide some tentative answers to this problem by analysing in what extent, in our particular example, it is true.
The port based modelling approach implies the use of the basic thermodynamic axioms. So the intensive or extensive nature of thermodynamics variables is thoroughly used. It leads to write the entropy balance, to formulate the irreversible entropy production term and to rewrite the constitutive relations in such a way the intensive variables are expressed as function of the extensive one.
The intensive variables encountered in thermodynamics are the temperature, the pressure and the chemical potentials of components of the systems. The extensive ones are the entropy, the volume and the mole number of each specie. The extensive variables are not classically used by chemical engineers to describe the process. Instead the measurable variables such as the temperature, the pressure and the mole numbers and generally the energy balance are used. These models are in general not reusable and a slight modification of hypotheses of functioning leads to a complete rewriting of the model.
A third consequence of the port based modelling is the rewriting of the kinetics rates in function of its conjugate variables, the forward and reverse affinities, instead of concentrations of reactants.
If bond-graph models are extensively used in mechanical or electrical areas, it is no more true in chemical processes and more precisely for chemical reactions. The bibliography is quite reduced in this domain. Our work is essentially based on the previous paper of Oster et al [2] et P. Breedveld [1].

In this paper, we provide a bond graph model of a complete chemical reactors using systematically the power conjugate variables. For chemical engineering this approach is novel in the sense that the elementary phenomena are represented as basic multi-port elements which can be locally connected.
The reaction under consideration is the gas phase balanced hydrogen – iodine reaction $H_2+I_2 \Leftrightarrow 2HI$.
The chemical reaction and the jacketed reactor in which the reaction takes place are modelled with the following assumptions:
- the constituent are perfect gas.
- the kinetics of the forward and reverse reaction satisfy the hypothesis of mass action constitutive relation .
- the reactor is continuous and perfectly stirred.

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EFFICIENT LINEARIZATION PROCEDURE FOR THE ACTIVATED SLUDGE MODEL NO. 1

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Due to stringent effluent norms the design, modeling, optimization and control of biological wastewater treatment systems (WWTPs), with as most representative example the activated sludge system, has gained a lot of importance during the last decades. To bring existing WWTPs in compliance with the present effluent norms, model based retrofitting and control offers a challenging perspective.
On the one hand, several *data driven* models for wastewater treatment plants have been proposed such as ARMA (AutoRegressive Moving Average) models, stochastic time series models and neural network models. They rely on input/output data without taking into account any prior mechanistic knowledge. The major disadvantage of these *black box* approaches is their lack of extrapolative power.
On the other hand, model development in the field has focused on *knowledge driven*, first principles models (i.e., *white box* models), such as the well known Activated Sludge Models (ASM) incorporating the basic biotransformation processes of an activated sludge wastewater treatment plant.
Although the ASM1 model (Henze et al., 1987) is commonly regarded as a state-of-the-art, mechanistically inspired model, its highly nonlinear and complex nature limits the straightforward implementation in optimization and control schemes. Since the latter are well developed for linear models, a linearized version of the ASM1 model would be highly advantageous. However, given the time-varying influent with respect to flow rate and load, a WWTP can never be regarded in steady-state due to which a linearization around a single equilibrium point is not realistic.
Therefore, we propose a *multi-model* approach (Murray-Smith and Johansen, 1997). The global operating range of the plant is partitioned in subdomains (according to temperature, incoming flow rate and recycle rate ranges) and for each subdomain a (locally valid) linear model is developed. The globally valid model is then a (weighted) sum of these local models (Smets et al., 2002).
This paper focuses on the linearization part of this multi-model strategy. A classical Taylor series expansion based linearization is compared with a newly developed linearization technique.
The here proposed approach retains all linear structural elements present in the original ASM1 model while the nonlinear (kinetic) expressions are approximated by (a limited number of) constant parameters. These parameters have to be identified on the basis of realistic input/output data. Such data sets are in this work generated with the configuration proposed by the COST 682 benchmark (`http://www.ensic.inpl-nancy.fr/COSTWWTP/`). The resulting model is a linear *grey box* state space model in the original state variables.
While the predictive power of both linear models turns out to be similar, the effort to obtain the linearized equation is not. Since the here considered system has 9 states and 10 inputs to be taken into account, a 9×9 Jacobian matrix and a 9×10 Jacobian like matrix have to be calculated to obtain the classical linearized model. Compared to this cumbersome task, the ease of generating the linearized equations with the new method (based on weighted linear combinations) is remarkable. Disadvantage of the latter is however that an identification procedure is required to obtain the values of the unknown parameters.

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APPLICATION OF THE PROCESS MODELING TOOL ProMoT TO LARGE–SCALE CHEMICAL ENGINEERING PROCESSES

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The application of the object–oriented process modeling tool ProMoT [1] to large-scale chemical engineering processes is presented. By the notion of large–scale systems we refer to plants that are made up of a large number of heterogeneous, highly integrated individual process units (see e.g. Fig. 1). It is shown that for the development of such large–scale process models the object–oriented modeling paradigm is particularly suited. This is due to the fact that by supporting a combination of bottom–up and top down modeling strategies ProMoT proves to be very flexible.
The classical example for bottom–up modeling is the process of modeling a distillation column that may be aggregated from more fundamental modules contained in a previously developed model library. Whenever a refinement of a more specific module is required a top–down modeling approach using the concepts of inheritance and refactorization seems most appropriate. All concepts are illustrated by means of an application of ProMoT to the modeling of an industrial scale process (Fig 1) [2].

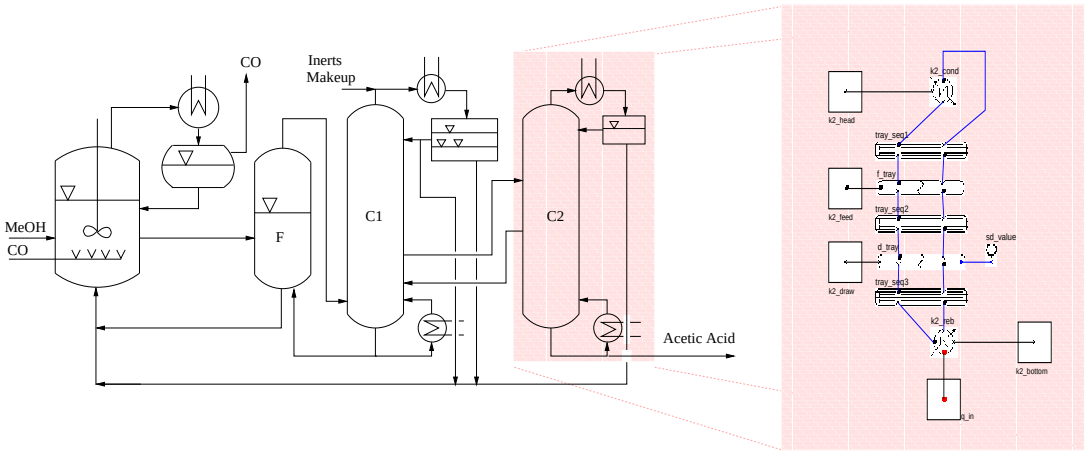

Figure 1: An excerpt of the overall flowsheet for the the production process of acetic acid with a zoom of the second distillation column indicating its decomposition and graphical representation in ProMoT.

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Modelling in Biopharmaceutics and Health Care

A NEW CLINICAL SOFTWARE PACKAGE for MULTIPLE MODEL (MM) DESIGN of DRUG DOSAGE REGIMENS for PLANNING, MONITORING, and ADJUSTING OPTIMALLY INDIVIDUALIZED DRUG THERAPY for PATIENTS

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Abstract. Dosage regimens based on parametric population models use single values to describe each parameter distribution. When a target goal is selected, the regimen is assumed to achieve it exactly. In contrast, MM dosage design is based on nonparametric (NP) population models. These have up to one set of parameter values for each subject studied in the population, each with an estimated probability. With this more likely population model, multiple predictions are possible. Using these NP models, one can compute the MM dosage regimen which specifically minimizes the predicted weighted squared error with which a target goal can be achieved.

When feedback from serum concentrations becomes available, each set of parameter values in the NP prior has its probability recomputed. Using that revised model, the new regimen to achieve the target with maximum precision is again computed. In addition, a new Interacting Multiple Model (IMM) sequential Bayesian method now estimates posterior densities when parameter values have been changing during the analysis, as occurs with acutely ill and unstable patients. These approaches have now been combined into a new Windows software package, the MM-USC*PACK programs, for clinical use. A three compartment linear model is used.

The library of population models currently includes Gentamicin, Tobramycin, Netilmicin, Amikacin, Digoxin, Vancomycin, and Trimethoprim. Carbamazepine and Carbamazepine Sustained Release are available for adults in the steady state, Carbamazepine with Phenytoin, and Carbamazepine with Phenobarbital for adults, in the steady state. There are also models for Valproate for both adults and pediatric patients, and Sustained Release Valproate for adults.

MODELING of NONLINEAR PHARMACOKINETICS of PHENYTOIN, and of CARBAMAZEPINE during its AUTOINDUCTION PERIOD

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Many antiepileptic drugs (AEDs) have pharmacokinetic (PK) characteristics that increase the risk for toxicity: relatively narrow therapeutic index, wide interindividual variability of PK parameter values, clinically significant drug-drug interactions. Because of the nonlinear kinetics of phenytoin (PHN) metabolism, and the autoinduction of carbamazepine (CBZ) metabolism at the beginning of therapy, therapeutic drug monitoring (TDM) and careful individualization of dosage regimens for these AEDs are especially important. Nonlinear models were developed to estimate the population pharmacokinetics of PHN (concentration-dependent Michaelis-Menten elimination kinetics) and of CBZ during its autoinduction period (time-dependent kinetics).

Population modeling was performed using the "Big NPEM" program and accessing the USC-NCRR Research Resource on the Cray T3E parallel computer at the San Diego Supercomputer Center. The model equations were written in Fortran source code, compiled, were incorporated with the patient data files and the appropriate instructions, and sent to the supercomputer, where the analysis was run. We have examined TDM data of 79 adult epileptic patients who received chronic PHN – monotherapy. Patient data files had only 2 to 3 measured serum levels, but some had 4-6 serum levels related to different dosage regimens. Estimated by the Big NPEM median population parameter values of PHN model (the rate constant of absorption (Kabs), the apparent volume of distribution (Vd), the maximum elimination rate constant (Vmax)) are in good agreement with those reported in the literature. The NPEM predictive performance evaluation shows the wide interindividual variability in patient response when all patient serum concentrations were predicted based on the population median parameter values. In contrast, the individual serum levels predicted on the basis of the median values of each patient's Bayesian posterior joint density gave good predictions for all subjects in the population. This Bayesian approach for PHN concentration prediction based on minimum non-steady-state TDM samples appears to be preferable to other steady state graphic methods and nomograms.

Although changes in CBZ kinetics during its autoinduction period (elimination rate is increased by a factor of approximately 2.5 during about 3-5 weeks of daily intake) are well documented, their magnitude varies among patients. We have described CBZ behaviour during the autoinduction period with a one-compartmental model with linear absorption. The main feature of this model is an asymptotic increase in the metabolic rate of elimination during autoinduction, starting from a preinduction value (D) before induction begins (λ), increasing asymptotically to a maximum value (D+A) after autoinduction is completed. The estimated (by Big NPEM) PK parameter values of D and (D+A) are in good agreement with those estimated in our population studies of pre- (0.018 ± 0.004 1/h) and postinduction CBZ metabolism (0.076 ± 0.067 1/h). For our 9 closely monitored patients, the mean value of ratio of post- to preinduction rate of CBZ metabolism was 4.5 ± 2.6 (CV=58%). When CBZ is started and the patient is titrated to a reasonable target goal, TDM and estimation of the individual parameter values may be helpful to determine the next step.

Bayesian feedback adaptive control and the proposed population models can improve AED dosage adjustment, can identify how close a patient is to the more saturated part of the PK curve, and can improve AED dosage for the individual patient.

PHARMACOKINETIC-PHARMACODYNAMIC MODELLING OF SIDE EFFECTS OF NITRENDIPINE

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Pharmacokinetics (PK) describes time courses of drug concentration in body fluids (mainly in plasma or blood) resulting from a certain drug dose, and pharmacodynamics (PD) describes the observed effects resulting from a certain drug concentration [1]. Mathematical modelling is regularly employed to study PK and PD processes.

The modelling aim in this study was to explore the relationship between plasma concentrations of a cardiovascular drug nitrendipine and occurrences of its side effects. The data were taken from a blind, randomised, four-way cross over bioequivalence study with a 20 mg single dose of nitrendipine. Forty young healthy men participated in the study. This way 160 plasma drug concentration - time profiles from 160 drug applications were obtained. During the study occurrences of side effects, their severity, onset time and duration were recorded. Overall, side effects occurred in 26 applications, headache in 24 applications, flush in 4 applications and vertigo in 1 application.

A time delay between maximum plasma concentration and appearance of headache was observed which resulted in a hysteresis in a side effect versus plasma drug concentration plot. PK/PD model for the incidence of headache as the main side effect was developed in two stages. For the PK part compartmental modelling was applied. A two-compartment model with lag time was determined as the best model to fit the observed plasma concentration data. The identified parameters of this PK model were used in the second stage to associate PK and PD data. An indirect model based on effect compartment (EC) was used as a link. The EC concentrations were directly linked to the incidence of headache by a fixed effect (logistic) model. The described PK/PD model was fitted to the side effects data. The estimates of k_{EO} (rate constant for distribution to EC), ec_{50} (effect compartment concentration at which probability of side effect appearance is 50 %), and n (slope in side effect versus concentration curve) were evaluated for each of the 24 applications. Nonlinear regression on data from all applications (with and without side effect) was used to find population estimates of the parameters. Evaluation of the model parameters revealed that incidence of headache is a consequence of increased sensitivity to nitrendipine concentration at the site of action.

However, it turned up that increased sensitivity to nitrendipine is not the only reason for occurrence of headache. Additional non-compartmental PK analysis demonstrated that incidence of the main side effect can be also explained by different nitrendipine disposition in the body. Comparison of the group with side effects and the group of applications without them confirmed that $AUC_{0\rightarrow\infty}$ (area under the plasma concentration curve), C_{MAX} (maximum plasma concentration), and $C_{MAX}/(t_{MAX} - t_{LAG})$, were significantly higher in the first group (t-test, $p<0.05$). Therefore it seems reasonable to conclude that appearance of side effects is also determined by increased extent and rate of absorption. Since more than thirty demographic, pharmacokinetic, haemodynamic, haematologic and biochemical parameters were known for each of the 160 applications, a multiple conditional logistic regression was performed in order to characterize the most influential parameters. $AUC_{0\rightarrow\infty}$, total concentration of plasma proteins, t_{MAX}, body height, plasma sodium and potassium concentration and change in diastolic blood pressure were recognized as significant parameters for appearance of side effects.

The developed methodology could supply useful criteria for the design of optimal drug dosage regimen, moreover it offers possibility for selecting individuals with high probability for adverse drug reactions.

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GENTAMICIN OTOTOXICITY: CHARACTERISTICS of PATIENT RESPONSE ANALYZED with SATURABLE MICHAELIS-MENTEN EFFECT MODELS.

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Abstract. We analyzed gentamicin pharmacokinetics (PK), and the amount and format of their therapy, in a group of eight patients who had developed clearcut vestibular toxicity from the drug. The results were compared with those predicted from a reference dosage regimen of 5 mg/kg once daily for 10 days. A linear PK model with both serum and peripheral compartments was used. There was overlap between the reference regimen and the toxic patients with regard to the total dose given per kg (but unadjusted for renal function), serum area under the curve (AUC), and the AUC in the peripheral compartment (both adjusted for renal function). However, when the serum compartment of the model was linked to a Michaelis-Menten saturable effect model, simulated relative drug uptake on phospholipids in vestibular, hearing, and renal tissues was used to evaluate the possible relative uptake at the vestibular effect site. The model results, using two different possible values of Km, separated all the eight toxic patients from the results seen with the reference regimen. This Michaelis-Menten nonlinear effect model may be of use in setting constraints upon aminoglycoside dosing regimens to avoid possible vestibular toxicity.

THEORETICAL MODEL OF TRANSMEMBRANE TRANSPORT OF SMALL MOLECULES CAUSED BY ELECTRICAL PERMEABILIZATION OF CELL PLASMA MEMBRANE

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Viability of the cell depends on integrity of its plasma membrane. The plasma membrane prevents exchange of substances between intracellular and extracellular space if they are not necessary for the viability of cell. The increase of permeability of the cell plasma membrane can be achieved by exposure of the cell to the electric field. In the state of increased permeability, the plasma membrane allows small and large molecules to be introduced into the cytoplasm. Phenomenon is transient and was termed electropermeabilization, often also named electroporation.

Electropermeabilization is widely used in various medical and biological applications such as electrochemotherapy, transdermal drug delivery and gene transfection, etc [1]. Efficiency of all these applications depends on parameters of electropermeabilization that influence transmembrane transport and thus the quantity of molecules that are introduced into the cells. With respect to this, optimal parameters for electropermeabilization have to be found to achieve best efficiency of the method.

In our study we present an upgrade of recently introduced model of diffusion-driven transmembrane transport of small molecules caused by electropermeabilization [2]. Our aim was to introduce number of delivered pulses as additional input parameter, since the existing model only uses two parameters pulse amplitude and pulse duration. Figure 1 shows the results that we obtained using the improved model. Nevertheless, the improved model still has certain problems with predicting the uptake at different pulses parameters than those shown here.

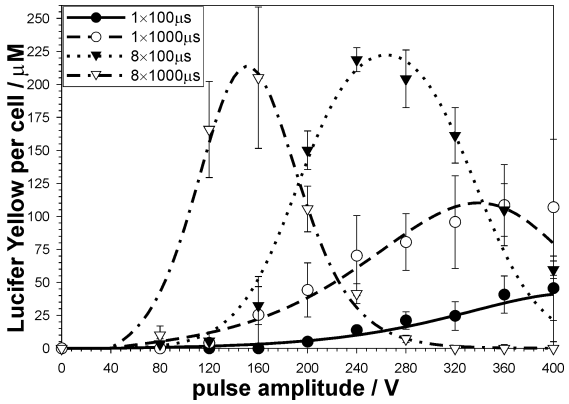

Figure 1. Results of modeling of uptake of Lucifer Yellow (LY) as a function of pulse amplitude U at different number and duration of pulses. The symbols represent experimental results (mean ± standard deviation) and the lines represents the course of uptake predicted by the model.

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COMPARISON OF METHODS FOR ESTIMATION OF PHARMACOKINETIC PARAMETERS FROM MEASURED DATA

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In pharmaceutical industry new drugs metabolisms and effects are tested according to the given time scheme. In the tendency of preserving as highest accuracy and reliability of experimental data as possible, there is a standardised doctrine that requires the use of unchanged - raw measurements data. From the measured data (the concentration of drug in the blood, blood pressure, heart rate etc…) in the given time scheme, the primary and secondary pharmacokinetic parameters are derived. Such derived parameters are the maximum drug concentration (in blood) (C_{max}), the time of occurrence of such concentration (t_{max}), the terminal decay slope of the concentration curve (β), and the area under the measured curve (AUC). Needless to say that the derived parameters from the measured data of poor accuracy can produce erroneous results.
Three methods for estimation of pharmacokinetic parameters from raw-measured data were tested. The first method ("direct method") is usually used for establishment of the maximum drug concentration in blood samples, for the time of occurrence of the concentration maximum, for the area under the concentration curve and some other parameters. At this method the measured data are used unchanged, without corrections of any kind. The second method fits the measured data to the analytical curve which is then used for further estimation of pharmacokinetic parameters. The originally measured data are replaced by the most probable function of pre-defined shape. The third method uses the measured data as the training set for the neural network. The time – concentration curve is learned and the relationship among the two parameters is then approximated by the neural network. Approximated data are then used for the estimation of pharmacokinetic parameters.
We propose that one of the two methods – curve fitting or approximation by the neural networks should be used. Perhaps it is best practice to use the approximation by the neural network. There are several facts that speak in favour to this method:

- It is simple to use and does not require a deep mathematical knowledge for end-user.
- It slightly corrects the coarse errors made by the presumptions that the maximum values for drug concentration in blood and the time of it's occurrence are necessarily among the values measured in fixed time points.
- The currently accepted "direct" method neglects the fact that the natural processes mainly depart from piecewise linear relationships. NNs introduce the smooth and non-linear function that approaches to the measured points with the given accuracy.
- The estimation of AUC (area under the concentration curve) is without doubt more precise then the one obtained by the trapezoidal integration of sparsely measured data. The integration uses non-linear function produced by the NN.
- The function approximation by the NN can be made by the relatively simple software solution where the number of measured data points are not fixed, nor should they be sampled equidistantly.

It is the matter of discussion, which method should be used as a standard, but as it is shown in our experimental work, the relative errors in derived data can be substantial. All three methods would have given almost identical results if the measured data would be without errors. The substantial differences between the results show that serious errors in measured data exist which can only be corrected partially. To use the raw data for further analysis is questionable practice.

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Manufacturing Systems

APPROXIMATE ANALYTICAL PERFORMANCE MODELLING OF A COMPUTER INTEGRATED MANUFACTURING AND MANAGEMENT SYSTEM

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Discussions with representatives of manufacturing enterprises has shown that there is a severe demand of prospective users for Computer Integrated Manufacturing and Management (CIMM) systems. On the other hand, large-scale suppliers of integrated management systems are not apt to be involved in the problems of manufacturing. Nevertheless, the market pressure will surely force development of CIMM systems. Considering that, research workers should anticipate the general structure of CIMM systems and investigate them in order to facilitate implementation of future solutions when they become available.

The paper presents the architecture of the System Media, being the reasonable initial step when developing the management and manufacturing in a big household appliance manufacturing enterprise. It is assumed that the feasible architecture of the CIMM system enabling to implement such integrated management and manufacturing will consist of a local-area network (of the Intranet type) and of a process-control oriented local area-network (e.g. LonWorks delivered by Echelon).
A question may be raised if individual users of the integrated system will be provided with a high enough throughput (especially for managerial users) or low enough round trip delay (especially for manufacturing unit users). To answer this question, it is necessary to model the future system since the CIMM system under discussion does not exist till now and no measurements on an actual system may be carried out.

The CIMM system under planning should be modelled as a set of users and service stations. On this set, there is stretched a net of closed loops (closed routes). This leads to the notion of the Kelly's networks. Unfortunately, there are not known accurate analytical methods for effective performance evaluation of the Kelly's networks [1] while the stochastic network performance evaluation methods are not useful for network designers [2]. Therefore, it was decided to use the method developed to investigate the first Polish wide-area network, the Inter-University Computer Network MSK.

The method used consists in writing the balance equations for the round-trip delay along individual closed loops (routes). This delay includes also the user's thinking time. The delays experienced by a packets at individual service stations passed by the closed loop (route) involved are assessed using approximations derived from the analysis of operation of networks with end-to-end acknowledgement and partially heuristic. The balance equations in their indirect form are solved by the iterative method..
The approximations were tuned and validated with accurate analytical models for configurations enabling accurate analytical modelling, with simulation using control system oriented simulation tool and by measurements carried out with the internal measuring tool Sitwa.

The approximate method proved to be very useful. The maximum error (determined by simulation and measurements) below 5% is better than good for actual system designers. The model may be used, as simulation, at each phase of the design process (e.g. when developing the general idea of the system). And it needs less than an order of magnitude of computer time than simulation. Application oriented models of various networks complete with software needed for for performance evaluation are available from the authors.

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COUPLING OF THE PRODUCTION PLANNING TO THE LOADS AND CAPACITIES ADJUSTMENT IN THE CONTEXT OF CONTRACT-ORDER

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Strong quality and delay requirements have catalyzed the emergence of new commercial paradigms, which have strongly modified the customer-supplier relationship. Companies frequently moved from the classical order between a customer and a supplier to the notion of a "contract-order" in which the supplier is linked with the customer through a delivery schedule with a forecast quantity for each delivery. They engage to deliver periodically products in varying quantities. These quantities can only be known exactly very late, "few days before the delivery", so they are faced with an enormous state of uncertainty in their load. This kind of order implies that the capacity must be flexible. So many flexibility levers should be used and prepared since long and/or medium term to be employed and well exploited in short term.

Classical models of planning operate in two different ways. The first one consists of carrying out, in medium term, production planning in a finite capacity way. So the load is adjusted to the capacity by smoothing the load in the time. The second one consists of performing, in medium term, production planning while ignoring capacity constraint (infinite capacity). Then the capacity is adjusted to the load in short term by using overtime and interim. Those classical models seem to be not efficient in the case of contract-orders for answering to the flexibility of the load, since in the first one the capacity is finite and in the second one the capacity adjustment is not integrated in the production planning.

A new approach is developed integrating the load and the capacity adjustment in the production planning and tending to satisfy needs and to offer flexible capacity, in an optimal way. The proposed approach consists of carrying out production planning while assuming a finite and variable capacity. Therefore, both the load and capacity are adjusted. The approach is based on the management of many flexibility levers (as overtime, interim and modes of functioning). Also, it allows order positioning to cover needs and decisions positioning to modify capacity. It is based on the resolution of a non-linear mathematical model to find an optimal policy for material and flexibility management.

This new model of planning allows companies to analyze in advance their capacity needs in order to guarantee their engagements with the lowest costs and to evaluate their risks. In fact, it allows companies to anticipate decisions and offers the possibility of a previous evaluation of costs and needs. So, they can check their arrangements to accomplish their contract-order.

FORECASTING OF LABOUR CONSUMPTION FOR REPAIRING OF AIRCRAFTS BY USING THE ARIMA MODEL

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1. Introduction

The methods of the ARIMA (Auto-Regresive Integrated Moving Average) model for forecasting of labour consumption for repairing of damaged aircrafts were presented. Information on labour consumption for failure removing of an aircraft given in the period of 10 years were used as basic data.

A loss of the technical features of aircrafts in relation to the ideal condition occurs with different intensity. Generally, it is a low-speed process to be observed only during many years' exploitation in routine tests, carried out according to an aircraft inspection program. The dominant problem is safety of aircrew and providing full readiness of machine at the military conflicts. Therefore, the matter of importance is to develop a support instrument for process of defining diagnoses.

At prevailing procedures every aircraft is submitted to regular inspections, and to repairs in case of failures. No problem appears, if the part to be replaced is stored in stock. The time consumption for services depends on the standards given in so called service logs. Because of quality of safety standards reducing the time consumption standard requirements for repairing is inadvisable. It is worth-while considering a possibility of forecasting of labour consumption for removing of damages for a few periods in advance. It would make it possible e.g. to define the number of staff needed for repairs.

2. Forecasting

The Fourier spectroscopic analysis for the investigated variable was carried out. A great discontinuity in series was recorded. The probable reason is that as far as three of four days are free of failure. The analyses done have demonstrated lack of seasonality. Some of results showed very low or equal to zero variancy, therefore it was impossible to make further significant analyses for these series.

For these reasons the aggregation of series into 1. month periods were done before analysis, with result of 122 one-month periods. The variable labour consumption was transformed by using the T4253H filtering method, summation and smoothing with the moving mean. The T4253H filtering method was used as giving the smoothed serie and allowing to retain characteristic features of original serie. The main aim of the smoothing methods was high-lighting of main systematic components of periodical serie by eliminating insignificant fluctuations (of random noise). A visual result of smoothing is transformation of the tooth-shaped linear chart into more smoothed curve. Next, the Fourier spectroscopic analysis of transformed serie was done. The highest values of periodogram were obtained for the period of 12. It is an evidence that the seasonality of the transformed serie of labour consumption was as high as 12 (1 year). The last 12 one-month periods were separated from accumulated data and the forecast started.

For forecasting the ARIMA methodologie developed by Box and Jenkins (1976) were used. The general model introduced by Box and Jenkins includes parameters of auto-regression and of moving average; it was put a differentiation operator into the model. The models are defined as ARIMA (p,d.q). Especially, there are 3 types of parameters: of auto-regression (p), of differentiation row (d) and, of moving average (q).

By subsequently increasing of p, d, q parameters, as well as by controling the significance of parameters and the function of the remainders autocorrelation, the allowable ARIMA models were presented. Next, the results obtained were compared with the real values (the last 12 one-month periods).

For the variable labour consumption forecasting was done by using the ARIMA model included in the STATISTICA 5.1. package.

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Robotics

STOCHASTIC APPROACH TO GENERATE APPROXIMATED ROBOT MODELS

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In context with the methods RRS (**R**ealistic **R**obot Simulation) and VRC (**V**irtual **R**obot **C**ontroller) one objective is to simulate the motion of industrial robots in real time [1]. The main problem is actually to establish and to solve the differential equation system of the robot dynamics (*direct dynamics*) in real time. Another application which uses the robot dynamics in real time is the method of model based control [2-3]. Here the *inverse dynamics* must be calculated during the sample time of the feedback controller. Direct dynamics (1a) and inverse dynamics (1b) are given in matrix form:

$$\ddot{\boldsymbol{q}} = \left[\boldsymbol{M}^*(\boldsymbol{q})\right]^{-1} \cdot \left[\boldsymbol{U}_S - \boldsymbol{b}^*(\boldsymbol{q},\dot{\boldsymbol{q}})\right] \qquad (1a), \qquad \boldsymbol{U}_S = \boldsymbol{M}^*(\boldsymbol{q}) \cdot \boldsymbol{r} + \boldsymbol{b}^*(\boldsymbol{q},\dot{\boldsymbol{q}}) \qquad (1b)$$

$\boldsymbol{q}$ is the $(n \cdot 1)$-vector of the time dependent n joint variables, $\boldsymbol{M}^*(\boldsymbol{q})$ has the dimension $(n \cdot n)$ and depends on the mass matrix and parameters of the actuation system, while the $(n \cdot 1)$-vector $\boldsymbol{b}^*(\boldsymbol{q},\dot{\boldsymbol{q}})$ is caused by gravitational-, centripetal-, Coriolis- and friction influences. $\boldsymbol{U}_S$ is the vector of the manipulated variables of the feedback control system, $\boldsymbol{r}$ represents a vector given by a control algorithm. In both applications it is not possible to use a complete model of the dynamics due to the high computational burden which is mainly caused by the calculation of the time variant system matrix $\boldsymbol{M}^*$ and vector $\boldsymbol{b}^*$ at each time step. This paper presents the software tool AGReMo (**A**utomatic **G**eneration of **Re**duced **Mo**dels). AGReMo is written in Matlab and generates an approximate efficient model with significant reduced computational burden without an essential loss in accuracy (Fig. 1a).

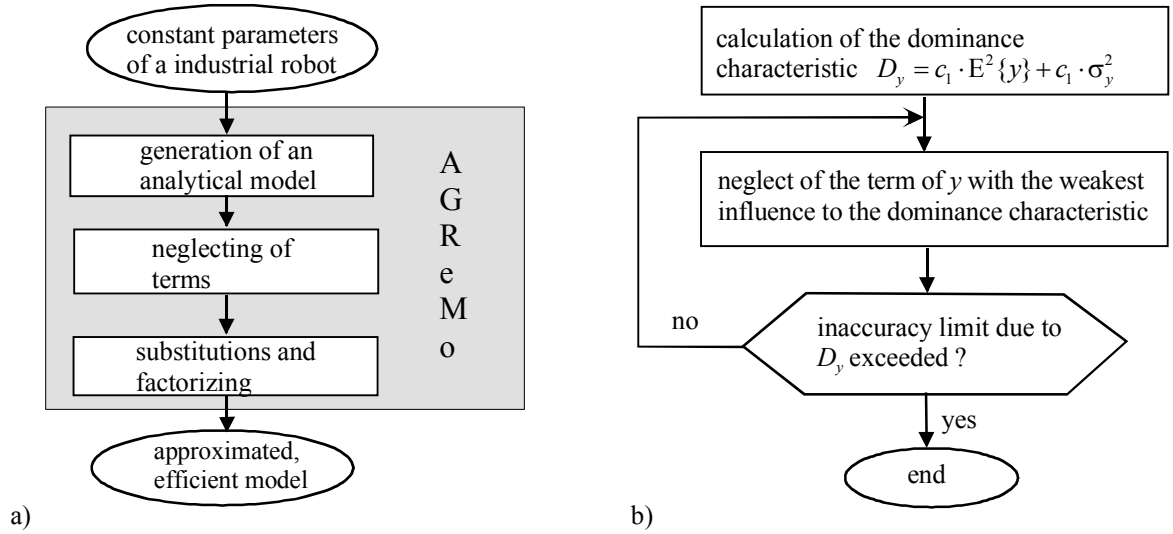

Figure 1: a) Matlab program system AGReMo, b) principle of neglecting terms of a matrix component

Basic idea for the neglect of terms is the consideration of robot motion state as probabilistic event. For example for any component y of $\boldsymbol{M}^*$ or $\boldsymbol{b}^*$ a dominance value D_y is calculated. D_y is based on the expected value and variance of y. Terms having a weak influence to D_y are neglected (Fig. 1b).
The application of AGReMo leads to reduced models with about 5% of computational burden related to the complete model without influencing significantly the model performance.

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MATHEMATICAL MODELLING AND OPTIMIZATION OF LINK-DRIVE MECHANISM FOR DEEP DRAWING MECHANICAL PRESS

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In this paper we present an optimization of a link-drive mechanism for a deep drawing mechanical press. The quality of products made with the deep drawing process is mainly influenced by their required shape and material. Among other technological parameters, such as friction contact and lubrication of the tool, the slide velocity is one of the most important. This velocity depends on press design parameters only. Each material has its optimal drawing velocity; therefore maximum drawing velocity is one of the deciding factors when selecting appropriate press. During last few years press manufacturers have begun to incorporate special link-drives into their presses. Their main advantage is much lower slide velocity during working part of the cycle, thus such presses can operate at higher operating speeds than conventional versions. The existing design of a link-drive taken into consideration has proved unsatisfactory; therefore optimization of the drive is necessary. Our intention was to achieve the required velocity characteristics in a defined area of movement. The final objective of the optimization process is to find such dimensions of link-drive members that the given requirements are satisfied in the best possible manner.

The drive (figure 1) consists of eccentric driving gear (R_4), connected to a coupler link (R_3-R_5). One side of coupler link is connected to the press frame via an additional link (R_2), and the other end is connected to an output slider-link combination (R_6-S). Mechanism is a 6-bar slider-crank mechanism and it is a modification of a standard 4-bar slider-crank version. A modified velocity characteristic (lower velocity in working part of the cycle) is achieved through extended coupler link and its connection to the press frame. Mathematical model is made and kinematic analysis is carried out in two steps: a) analysis of the 4-bar mechanism (R_1-R_2-R_3-R_4); b) analysis of the 4-bar slider-crank mechanism (R_4-R_5-R_6-S), where the output results of the first analysis are the input data for the second one.

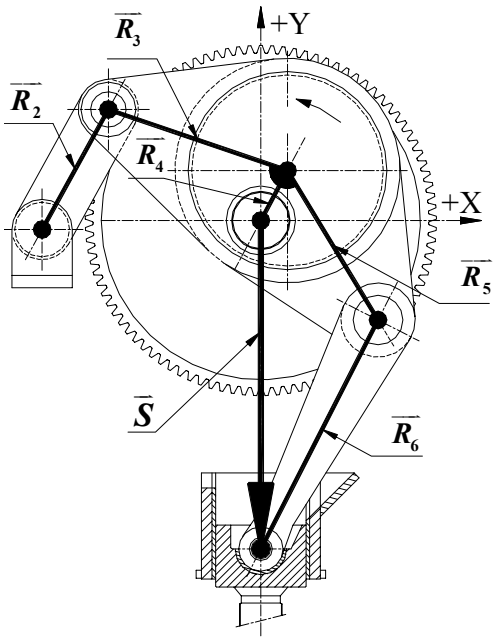

Figure 1: Deep drawing mechanical press link-drive

The relationship between input and output link is non-linear, therefore non-linear optimization procedure is used. Because the whole process is time-dependent it cannot be used directly in the standard optimization algorithm but has to be transformed into a suitable form instead. For this task the method of artificial variable is used. The optimization algorithm is based on the method of sequential quadratic programming (SQP). We used the NAG FORTRAN library of numerical algorithms. Current design of the drive was starting point for the optimization. The cost function chosen for optimization was maximum absolute acceleration of the slide. Task is to minimize this acceleration as possible and by doing that to stay within required constraints.

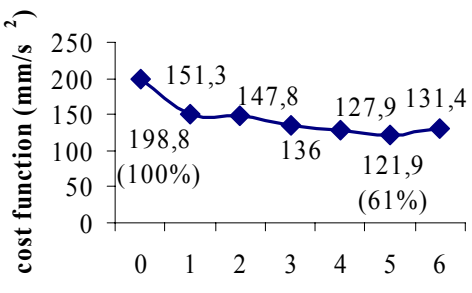

Figure 2: Optimization history

Figure 2 represents optimization history of the given problem. The cost function was minimized on approx. 61% of original value, so optimization was successful. Slide velocity in the working part of the cycle is lower and more constant than with original drive. The area of constant slide velocity is also extended; therefore more time is available for material to yield and deform during the drawing process. Proposal for further work is to incorporate dynamics (operational forces, joint forces, etc.) and perform additional optimizations.

A GENERALIZED MODEL FORMULATION FOR MANIPULATORS WITH FLEXIBLE LINK(S) AND JOINT(S)

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Lightweight robot manipulators, where the arm is made of composite or other materials with a relatively low mass, are attractive because energy consumption during operation is reduced and a heavier payload can be carried compared to conventional robots of a similar size. However, an unavoidable consequence of the lightweight design is that the links have significant flexibility. Because of the interaction between rigid and flexible motions, the resulting dynamic equations of flexible manipulators are highly complex and, in turn, the control task becomes more challenging compared to that for rigid robots. Therefore, a first step towards designing an efficient control strategy for these manipulators must be aimed at developing accurate dynamic models that can characterise the above flexibilities along with the rigid dynamics. Whilst a significant amount of research has previously been carried out with the aim of developing accurate models of flexible dynamics, the majority of this has been concerned with modelling a single flexible link. This is of little benefit in formulating a model of a flexible manipulator, where at least two links need to be flexible in order for the manipulator to have any practical use. Where two flexible links are jointed together, there is a significant amount of coupling between the link dynamics that is completely ignored in single-link models. To further complicate matters, there is flexibility in the actuated joints of manipulators that becomes particularly relevant when modelling a system of two flexible links. Whilst some past research has addressed the issue of modelling a coupled system of two flexible links, there has very little work that considers joint flexibility at the same time except for one paper [Gogate 1993], but this made simplifying assumptions. In response, this paper describes the development of a new generalised model formulation for flexible multi-link manipulators that considers both link and joint flexibility and avoids approximations made in alternative modelling approaches. Emphasis is placed on maintaining generality in the model so that it can be applied systematically to manipulators with any number of flexible links. Simulation results demonstrating various aspects of the model are included in the full paper. As an example, the figure below illustrates the improvement when the approximations made by Gogate are avoided.

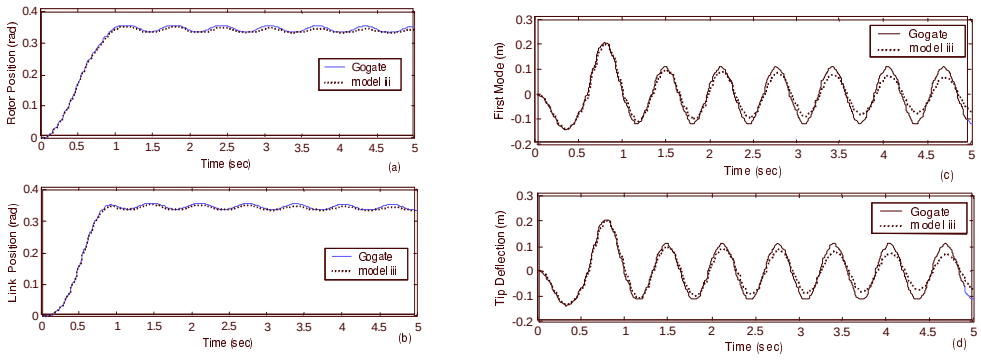

Figure: Comparison of the generalised model with Gogate's approximated model

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MODELLING AND VALIDATION OF FLEXIBLE ROBOTIC LINKS

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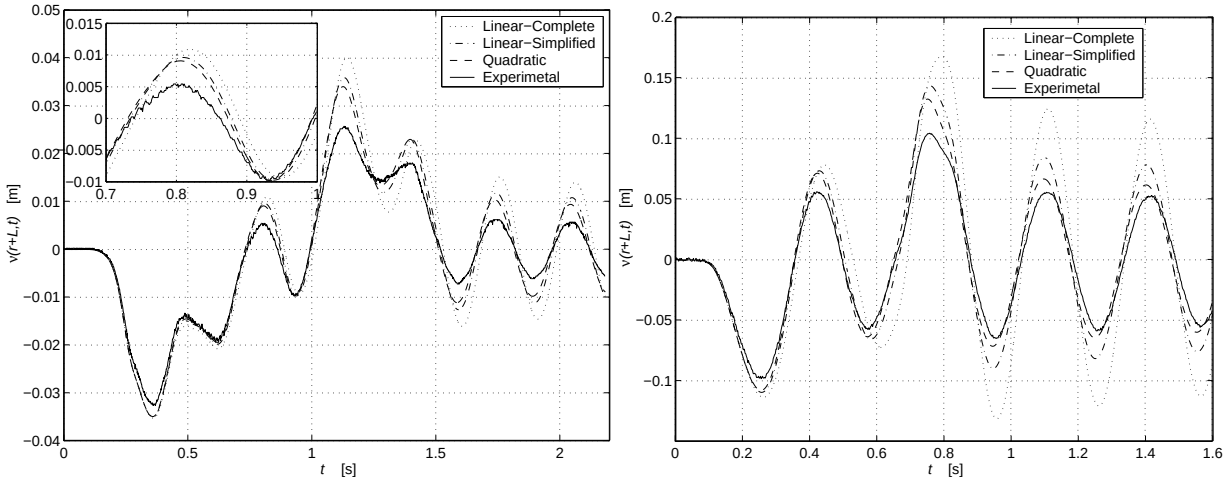
This work treats the problem of modelling and model validating the mechanical deformation in light-weight robotic manipulators. The dynamic behavior of a flexible link undergoing large and fast *rigid body* rotations is modelled. The modelling problematic is presented starting from common linearizing approaches found in the related literature. It then evolves leading to a nonlinear dynamics model capable of capturing the beam stiffening due to the centrifugal forces induced by the fast joint rotations. This model is founded on two basic assumptions: inextensibility of the neutral fiber, and moderate rotations of the cross sections in order to account for the foreshortening of the link due to bending. Simulation and experimental results show that the latter model has the closest dynamic behavior to the real link. The experimental results are obtained by measuring the tip displacement of the link with a fast image acquisition system. The contribution of this work is thus twofold; first, the differences between linear and quadratic models at the partial differential equations level are presented, and then model results are set against experimental data obtained from a laboratory prototype. The novelty in the contribution resides in the experimental confrontation between the experimental data and the simulation results at different joint velocities, which was possible through the use of a high speed image acquisition system that allows the direct measurement of the tip displacement in real time (1000Hz). Furthermore, the modelling approach and analysis, provides a framework for modelling flexible manipulators aiming at control.



a. $\theta_{max_{ref}} = 6\,\text{rad/s}$ b. $\theta_{max_{ref}} = 8\,\text{rad/s}$

Figure 1: Tip displacement for $\theta_{max_{ref}} = 6\,\text{rad/s}$ and $\theta_{max_{ref}} = 8\,\text{rad/s}$

Acknowledgements

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Applying Models in Process Industries

UML Specification and Development of Safety-relevant Industrial Communication Systems

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Abstract

More and more safety-relevant applications are being handled within industrial automation. The IEC 61508 standard describes requirements of functional safety and according development processes. Micro processor based device solutions for safety-relevant applications are faced with this standard. This forces the device manufacturer to contact third party partners such as TÜV and BIA which verify the development process and the development result. This causes a resource overhead by the device manufacturer. Therefore, these manufacturers are looking for design tools with round trip opportunities. The basis for these design tools is the Unified Modelling Language (UML) that has to be specialised by design guidelines to fulfil the requirements of software development of functional safety systems.
This paper shows the necessary steps from a formalised UML specification of a PROFIsafe specification to an implementation in a field device. The procedure of deriving software out of an UML-CASE tool and its verification and integration into a safety-relevant environment will be described.

Keywords: Safety, UML, Embedded Systems

Semantics of the Phase Model of Production: Application

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This article deals with the semantic aspects of the visual description language *Phase Model of Production* (abbreviated herein as PMP) [3], which is used in the area of Process Control Engineering.

The development, or realization, of process control solutions demands a sufficient detailed knowledge about the processes to be controlled. The means generally used for the design of such solutions often do not satisfy this demand. Therefore, a more qualified description means for processes has been sought after since the middle of the 70's. During this time, according to the phase-oriented model of "Software Life Cycle" [1], M. Wienand initially named the term *Phase Model of Production* (one can find references in [3]). The starting point for the Phase Model of Production as a semantic process description is the basic flowsheet according to [2]. In general, the PMP is a graphical, partially formalized form of description for – not only, but mainly – production processes. Because of their plausibility and simple structure, PMPs can be used as a basis for discussions with all people involved in the planning process, even and especially if they come from different fields of industry.

Previous papers about the PMP (e.g. [3],[4],[6]), describe, among other things, the application of this description language for various kinds of processes – nevertheless, they do not handle the different semantics which result nor the different network structures arising from this in detail. Furthermore, as in most visual languages in a software-engineering context, there is a lack of a formal basis for the PMP, especially if it should be used as an input for simulations, or as a source for automatically generating code. For these reasons, the Institut für Softwaretechnik (University Koblenz-Landau, Germany) and the Lehrstuhl für Prozessleittechnik (RWTH Aachen University, Germany) started to set up a strictly formal description of the different possible semantics of the Phase Model of Production. In this first step, the formalization only applies to the primary structures of the PMP; enhancements like energies [5] or technical resources are not considered. This article shows some of the basic thoughts on this work, whereby the formal description of these semantics will be explained in detail in a separate article by Martin Schulze and Jürgen Ebert [7].

After a description of the basic structure of the Phase Model of Production, a short classification of the processes to be considered is given. Based on this, an analysis of the possibilities of the description of pure batch and pure conti processes with PMP graphs follows, with simple examples given. Additionally, aspects of information flow, network structures and buffering of product states in the presented 'PMP styles' are discussed.

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Semantics of the Phase Model of Production: Formalization

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Abstract

In this paper it is shown how a method to formalize the semantics of visual languages in software engineering can be applied to a visual language in process control engineering, nameley the "Phase Model of Production" (PMP) [1].
Syntax and semantics of most visual languages are not formally defined. For example the meaning of PMP diagrams is only described in natural language. But to use diagrams in a contract or in an instruction or to implement tools, a concrete semantics is necessary to define which diagrams are valid and what is their meaning.
In this paper, a formalism already successfully applied to visual languages in software engineering [2], [3] is used to define semantics for PMP diagrams. In this approach class diagrams and constraints in a $\mathcal{Z}$-like formal notation (EER/GRAL) [4] are used as metamodels to define the syntax of visual languages. Then, the semantics are defined operationally by abstract automata defined in $\mathcal{Z}$ that make use of the syntax description.
We show how different views on PMP diagrams [5] can be formalized using this approach.

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A Metamodel for generic data exchange between various CAE Systems

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In the article a metamodel is introduced and shown for the structuring and categorisation of CAE planning data, how on the basis of such a model the life-cycle-accompanying exchange of planning data between the different systems involved can be generally organised.

The planning process is typically a strongly distributed process, in which a multiplicity of different planners and working groups are involved. Depending upon craft, planning phase or assigned organisational unit the planners use on their own environment optimised CAE systems. Efforts of the users to standardise this tools showed that this is only reasonable and possible up to a certain degree. Also the efforts of the manufacturers to solve the total task by an integrated proprietary system appears a little promisingly. A cause for it are not only the multiplicity of different procedural models, preferences of the involved groups or the diversity of the objects which can be specified, but above all the indeterminable complexity of the application models and aspects. At that background a comprehensive integrated application model seems not to be realisable. Such a model is however a precondition for a uniform file or a standardised exchange of planning data. Thus the question arises through renouncement of a standardised application model, how the exchange of planning data can be organised, in order to ensure universal DP-technical information flow during the engineering process and over the entire life cycle of the plant.

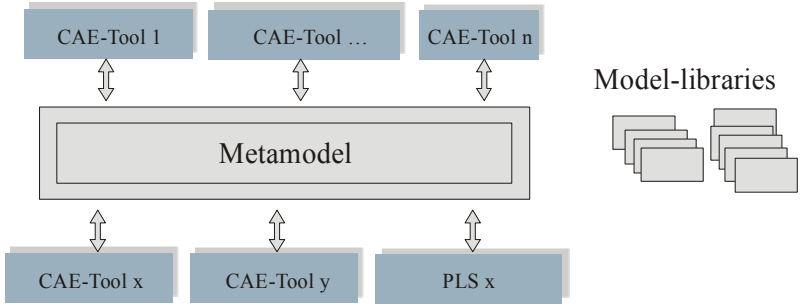

Figure. 1: Data exchange on basis of a generic metamodel

In the article a generic data model is presented, that can be used as a middleware between different CAE systems. The presented model does not define concrete plant elements with concrete attributes. It describes rather a metamodel for the creation of different plant models.

Characteristic of the metamodels are:

- A uniform modelling of arbitrarily complex plant elements by the definition of a metamodel
- Object-oriented modelling of plant structures
- Summary of plant elements in libraries.

The metamodel is developed in co-operation between ABB and the chair of process control. With the goal of a direct communication between various CAE systems the metamodel is described as XML schema.

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Biology

A honeybee population model with special emphasis on resource management and division of labor

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We here present a mathematical model of the population dynamics of a honey bee colony. The model allows daily predictions of the number of bees and brood as well as of the amount of resources stored in the combs under various conditions throughout a full year. The model incorporates several aspects of honeybee ecology like task partitioning and division of labor. It is formulated in a way that one can easily query the colony's response to bee keeping treatments and scientific treatments applied to the colony. It also allows to study the effects of several environmental factors onto the population dynamics of the modeled colony and onto its collective behavior.

Eusocial insect colonies, which have only one reproductive female show characteristic population dynamics, which can be described best by using mathematical modeling. They differ significantly from the population dynamics described by classical ecological models, which deal with populations consisting of all self-reproducing individuals. The intrinsic reproduction rate of the honeybee queen follows a typical season-dependent time pattern, which would result in an easy to predict colony development. What turns this system into a complex one is the fact that many feedback loops regulate the viability of the produced brood.

The amount of effectively surviving brood is collectively regulated by worker bees (via cannibalism and cell preparation) according to the current food supply and to the current food demand of the colony. The colony is characterised by division of labor, the details of which are influenced by demography and by colony demands. The colony is able to maintain internal homeostasis (e.g. a stable nest climate) and to react to disturbances with plasticity. Internally triggered events like swarming and external events like bad weather periods can cause severe changes in the age structure and in the food storage situation of the colony. Our model is intended to predict both: the reaction to gradually happening environmental changes and the reactions to sudden events like swarming.

The model is implemented by a set of difference-equations, which calculate daily changes in the status parameters of the colony (e.g. number of brood, number of bees, ...). In simulation runs, values are retrieved in discrete time steps of one day. The model consists of several linked subsets of equations, each modeling several aspects of a honeybee colony: "development and aging of bees", "mortality", "task selection", "resource allocation", "environmental influence", and "space".

We performed simulation runs with “optimal” weather data and with real weather data. Both kinds of simulations predicted a colony development pattern as depicted in literature. Also the pattern of pollen collection matched our experimentally collected data, especially during longer periods of rainy days.

We performed sensitivity analysis with real weather data and with “optimistic” weather data ("optimistic" means: no rainy days and no cold days except in winter). We randomly sampled configuration parameters within a range of ±25% from our base model configuration. Both methods showed that our model’s predictions have a high stability. When we configured the model for small hive sizes (low total cell number), our analysis revealed a change in model behavior as soon as the simulated combs were almost filled up with brood and food. There is obviously a competition between honey and brood for the remaining empty cells. Further analysis of scaling solely the egg laying rate from 500 eggs/day to 2500 eggs/day showed that there is an optimal intrinsic egg laying rate which depends on the available space and on the average foraging activity.

We think our model provides a valuable insight into the relationships between honeybee population dynamics and space and resource regulation. This makes it very useful in judging the implicit effects of the colony treatments we usually perform during our behavioral experiments with real bees.

MODELLING FRUIT CHARACTERISTICS DURING APPLE MATURATION: A STOCHASTIC APPROACH

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During apple maturation several fruit characteristics, such as firmness, colour, stage of starch transition, components of taste (e.g., soluble solid content) are measured to follow the evolution of ripeness and to determine the optimal picking date. After harvest apples are stored under cold and controlled atmosphere conditions to retard the respiration metabolism and to guarantee good product quality for further commercialisation. Since its large economic impact on growers business and fruit marketing it is important that the optimal picking date as well as changes in fruit quality attributes after harvest can be predicted as accurately as possible.

In recent years many mathematical models have been developed to predict the change of fruit charactersitics during maturation and cold storage. Instead of modelling the full chain of underlying biochemical processes, typically models of minimum complexity are developed to describe the basic dynamics of fruit quality attributes by means of a limited number of state variables. However, these models are deterministic and do not take into account the large natural variability of fruit quality attributes.

In this work present methodologies for modelling fruit charactersitics during apple maturation are extended to account for the huge variability which is observed during the growing season. The large differences in fruit characteristics at a given time instance mainly originates from biological variability, and variability in the physiological stage of fruit, environmental conditions and subjective measurements. The evolution of fruit quality attributes is represented by means of a system of differential equations in which the initial conditions and the model parameters are specified as random variables together with their probability density functions.

Two methods are investigated to assess the propagation of the probability density function of fruit characteristics over time: (i) a straightforward Monte Carlo method, and (ii) a methodology obtained from stochastic systems theory. It is shown that the applicability of the Monte Carlo method is limited because of the large simulations which are required to bound the statistical estimates of the transient probability density function within reasonable limits. Stochastic systems theory provides two alternative methods to compute the propagation of probability density functions through systems described by differential equations (Melsa and Sage, 1973). A first one is the variance propagation algorithm which computes a first order approximate solution for the mean and the covariance of fruit quality attributes. A second, more fundamental, approach considers the solution of the Fokker-Planck equation. Because the Fokker-Planck equation is a partial differential equation of hyperbolic type, usually its solution can not be derived in closed form. Numerical tools were developed to discretise the computational domain and are based on finite difference schemes. The evolution of soluble solid content during apple maturation was chosen as an illustrative example to demonstrate the main features of both methodologies.

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CRITICAL EVALUATION OF A NONLINEAR MODEL FROM PREDICTIVE MICROBIOLOGY USING SENSITIVITY ANALYSIS AND OPTIMAL EXPERIMENTAL DESIGN

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Reliable system identification requires accurate model structure characterisation and parameter estimation. Experimental data used in this process must be rich in information on the (bio-)process dynamics. When the model structure has been characterised, the methodology of optimal experiment design for parameter estimation can be addressed for unique and accurate parameter estimation. Parameter identifiability is closely related with the model output sensitivity, i.e., the model output changes induced by (small) parameter deviations. Inputs with large model output sensitivities are highly informative in the context of parameter estimation.
In this paper, the model structure and the parameter estimation problem of a four-parameter nonlinear model from predictive microbiology are critically assessed on the basis of a model output sensitivity analysis and optimal experiment designs for parameter estimation. The four-parameter model under study is the so-called cardinal temperature model with inflection point and relates the microbial specific growth rate with environmental temperature [1].
In general, a model output sensitivity analysis may unveil *hidden* model structure shortcomings. Here, it is shown that at certain temperture input levels, specific growth rate predictions are (theoretically) perfect, i.e., carry no uncertainty. Given the field of application, this observation raises the matter of awareness when using this model for prediction purposes.
During optimal experimental design, optimal temperature input placement within region of model validity is at the order. Different design criteria based on the Fisher information matrix are applied [2,3]. Opposed to equidistant spacing of temperature levels which is common practice, replicate specific growth rate determination at four optimally selected temperature levels is more informative with regard to accurate parameter estimation. These four temperature levels are close to the maxima of the sensitivity functions which implies a moderated model nonlinearity at the level of the model parameters. Besides the classically used criteria focussing on parameter estimation accuracy, a criterion aiming for minimum prediction errors is considered. These so-called G-optimal designs are quite distinct from those based on (common) parameter-related design criteria, and yield indeed the lowest prediction error.

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DEVELOPMENT AND ANALYSIS OF A NOVEL CLASS OF PREDICTIVE MICROBIAL GROWTH MODELS

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Single species microbial growth, whether in a bioreactor or in a food product, normally passes three phases: first a lag phase during which the microbial cells adapt to their new environment, followed by an exponential phase during which the cells multiply exponentially, and finally a stationary phase in which the maximum population density is reached. Growth is a self-limiting process principally due to either (*i*) the *exhaustion* of *one of the essential nutrients* or (*ii*) the *accumulation* of *metabolic waste products* which inhibit growth [3]. Most models used in predictive microbiology do not consider this microbiological knowledge [1]. This is illustrated with the nowadays widely used growth model of Baranyi and Roberts [2]:

$$\begin{aligned} \frac{dN}{dt} &= \left(\frac{Q}{1+Q}\right) \cdot \mu_{max} \cdot \left(1-\frac{N}{N_{max}}\right) \cdot N \qquad \text{with } N(t=0)=N_0 \\ \frac{dQ}{dt} &= \mu_{max} \cdot Q \qquad \text{with } Q(t=0)=Q_0 \end{aligned}$$

The first differential equation describes the evolution of the microbial load N [CFU/mL]. The *adjustment function* $Q/(1+Q)$ describes the lag phase by means of the physiological state of the cells Q [-]. The latter is assumed to be proportional to the concentration of a (hypothetical) critical substance which is the bottle-neck in the growth process. The second factor expresses the exponential phase, with μ_{max} the maximum specific growth rate [1/h]. The *inhibition function* $(1-N/N_{max})$ describes the transition to the stationary phase with the maximum microbial load N_{max} [CFU/mL]. The second differential equation describes the exponential evolution of Q. Remark that the *adaptation function* can be regarded as mechanistically inspired, whereas the logistic-type *inhibition function* is purely empirical [3] as it does not include any cause-effect relationship. In this research a novel class of mechanistically inspired, and modular extendable models is constructed, analyzed and compared to the model of Baranyi and Roberts. The global model structure consists of a general expression for the microbial evolution

$$\frac{dN}{dt} = \mu_Q(Q) \cdot \mu_{max} \cdot \mu_S(S) \cdot \mu_P(P) \cdot N$$

together with the appropriate differential equations for the physiological state Q [-], the substrate S [M] and the toxic product P [M]. The first factor $\mu_Q(Q)$ accounts for the lag phase and is equal to the *adjustment function* of the model of Baranyi and Roberts [2]. The second factor describes the exponential growth with maximum specific growth rate μ_{max} [1/h]. The third factor $\mu_S(S)$ describes the influence of the substrate concentration S on the microbial evolution, e.g., as a Monod type relationship. The fourth factor $\mu_P(P)$ accounts for the inhibition of microbial growth by a toxic product P. Thorough analysis and model fittings on a large set of experimental data indicate that the novel model types show equal fitting capacity in comparison with the model of Baranyi and Roberts. However, the mechanistically inspired incorporation of the effects of nutrient exhaustion and/or toxic product accumulation makes the novel model class more convenient for application in more complex, yet realistic situations, e.g., microbial interactions where microbial growth of a pathogen is inhibited by lactic acid produced by lactic acid bacteria or growth in structured media where the effect of a limited diffusion of nutrients and/or toxic products might play a key-role.

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EVALUATION OF ADDITIVE AND SYNERGISTIC PREDICTIVE MODELING: APPLICATION ON FUNGAL INACTIVATION BY COMBINED TREATMENTS

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Micro-organisms like bacteria or fungi display a remarkable diversity and adaptability, making them able to colonize almost every conceivable niche on earth. Given their dynamic nature and the relative scarcity of mechanistic knowledge underlying cellular processes, it is not surprising that unexpected observations can be made when exposing micro-organisms to fluctuating environmental conditions like, e.g., temperature. Often, these observations can not directly be related with the respective behaviour under static environmental conditions. This not only holds for conditions where micro-organisms can multiply or survive, where stress-related responses come into play, but also for lethal (inactivating) conditions, where sequential/combined treatments can enforce each other (*synergism*), be neutral (*additive*) or counteract each other (*antagonism*).
In order to ensure *microbial food safety and quality*, a range of more classical growth inhibiting or inactivating treatments (e.g., lethal temperatures, low pH, low water activity, disinfecting detergents, ...) or recently explored alternative techniques (e.g., ohmic heating, pulsed electric fields, pulsed light, ...) are currently in use or under development. As mechanisms underlying these inactivating treatments are only partially unraveled, it is most often not possible to *predict* synergistic, additive or antagonistic effects of combined treatments based solely on observations for the single treatments and associated modeling approaches.
In this research, the sequential mild heat and pulsed light treatment of the fungi *Botrytis cinerea* and *Monilinia fructigena*, two important fungi with respect to postharvest losses of strawberries and sweet cherries, are under study. The aim is to evaluate the suitability of a purely additive predictive model for a combined treatment, as based on modeling approaches for two treatments separately. Hereto, an inactivation model relating the population of fungi N log-linearly with time t making use of a first-order inactivation constant k_{max}

$$\frac{dN}{dt} = -k_{max} \cdot N \tag{1}$$

for the mild heat treatment is combined with a sigmoidal model for the pulsed white light treatment

$$\frac{dN}{dt} = -k \cdot N \quad \text{where} \quad k = k_{max} \cdot \left(\frac{1}{1+C_c}\right) \cdot \left(1 - \frac{N_{res}}{N}\right)$$

$$\frac{dC_c}{dt} = -k_{max} \cdot C_c$$

where an initial delay in the inactivation (a so-called shoulder) is related with $C_c(0)$ and a sub-population which is not inactivated (N_{res}) is incorporated. After the introduction of an *Interaction Factor*, linearly related with the temperature and duration of the heat treatment, a synergistic/antagonistic modeling approach is developed, enabling the accurate prediction/description of the fungal evolution as influenced by the sequential treatment with mild heat and pulsed white light. Synergism is observed for a rather severe heat treatment (high temperature and/or long treatment duration) followed by the pulsed white light treatment and could possibly indicate a complementarity in lethal actions on microbial/biochemical level. Antagonistic effects are visualized when using a very mild heat treatment, indicating possibly the alteration of the microbial cells to a more stress resistant state.
Acknowledgements are presented in the Full Paper associated with this Abstract.

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TOWARDS DNA CHIP ANALYSIS AND DISCRETE TOMOGRAPHY BY INVERSE PROBLEMS AND OPTIMIZATION

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Many problems in computational biology and bioinformatics need a new combination of methods of discrete optimization and continuous nonlinear optimization. Motivated by the concrete example of protein folding we pay attention to such a structural frontier. We mainly concentrate on new theoretical and constructive-practical interpretations of discrete tomography and inverse problems. Protein folding is one of the fundamental unsolved problems in molecular biology. A protein must assume a stable and precisely ordered confirmation to perform its biological function properly. Although much is known about the structural details of that native folded conformation of proteins, very little is examined about the actual folding process. For an understanding of protein folding has important implications for all biological processes, including protein degradation, protein translocation, aging, and human diseases, there is great interest in a deep understanding of the structure. In the following we present an approach which is based on discrete tomography and inverse problems. A traditional motivation of our *inverse problem* from discrete tomography comes from quality control in VLSI design. It demands *homogeneous* crystalline layers consisting, e.g., of silicon. Homogenity means "non-roughness" of a considered atom cluster which is discrete and three dimensional. We give the following model description, which will be extended for biological purposes at the end of the paper.
Suppose a set of atoms located on a chip. We want to measure the distribution of the atoms (represented as balls in a lattice) by "shooting" parallel electronic beams and recording the reflected "X-rays" at hyperplanes. How many directions of beams do we need, how to choose them? We embed our interest in three dimensions into the general case of finite dimensions d. The special situation of "convex" sets is comparatively well-understood; so, four suitable directions are enough for clusters in $\mathcal{Z}^d$, $d = 2$ The "nonconvex" situation, however, is much harder. Some authors represent a given or not given atom at some position by 0, 1 (or: blank, pixel, respectively) such that projection in reverse direction means addition of 1s. This case is of basic importance, because higher dimensional cases can be arranged in a rectangular planar way. Moreover, provided these sums being arranged as line or column sums of a binary matrix we are guided to allocations like combinatorial problems.
However, the choice of k directions remains a delicate matter, which can exploit any knowledge where 0s are lying. For a recent approximative algorithm in binary tomography and to literature on previous ones we refer to. In the following, we look at this practical motivation of concluding from discrete measurements to the unknown discrete cluster as an inverse problem of *"discrete → discrete"* type.

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Finite Automata

MODELING AND ANALYZING FINITE STATE AUTOMATA IN THE FINITE FIELD $\mathbb{F}_2$ [1]

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The investigation of the cyclic transition behavior is considered a major task within the analysis of finite state automata. Reminiscent of eigenvalues in linear continuous systems, linear state space models using *arithmetical polynomials* have been established for deterministic finite state automata in order to ascertain the cyclic structure of the state space by setting the eigenvalues of the closed loop system dynamics [1]. The main drawback of this approach is the lack of sufficient and efficient criteria for pointing out the existence of particular cycles. Even for linear systems this approach provides just necessary criteria such that for some fixed set of eigenvalues virtual cycles may occur. Another drawback is that the multiplicity of particular cycles cannot be investigated within this framework. Getting away with the latter problem a new method employing *Walsh functions* was introduced [4], so as to determine the cyclic structure of the state space, completely leaving aside the eigenvalues of the system dynamics and referring to the state equation only. The crucial disadvantage remains: the complexity problem, since solving for certain cyclic states is NP-complete. This originates from the fact that solving a linear diophantine system of equations for *boolean solutions only* (e.g. cyclic states) is on the class of NP-complete problems. There is no polynomial time algorithm that constructs boolean vectors out of a linear combination of integral or rational vectors. Hence, typical problems in practice, which usually comprise an enormous number of states, have to be considered intractable within these approaches. A further drawback is the missing implementation of input variables in the *Walsh function* framework. Thus neither of the approaches, *arithmetical polynomials* and *Walsh functions*, provides sufficient means of feedback design. A shortcoming, common in both models, is the lacking describability of non-determinism. In contrast to the latter, the model to be developed in this paper allows of an efficient cycle analysis for deterministic and non-deterministic automata and is capable of overcoming these obstacles using an algebraic state space description that is formulated strictly in (modulo 2-) operations on the set of boolean numbers, the finite field $\mathbb{F}_2$. Finite field models have already been under consideration in the control community [2]. However, neither were they utilized for determining the cyclic structure of automata nor were any analogies drawn to linear continuous systems. On the other hand concerning linear systems much of the theory was already developed as early as the sixties — for instance the design of linear feedback shift registers [3] — but has not been adapted for control purposes yet. In this contribution, based on the system invariants of a linear system, in particular the elementary divisor polynomials of the system dynamics, the finite field framework is shown to enable sufficient criteria for determining all cycles of a deterministic automaton (in multiplicity and length). As a consequence, the feedback design problem specifying the cycle structure of a controlled automaton becomes feasible[2]. In the general, multilinear case this can be done using Gröbner-bases[3]. Specially for linear systems of equations this kind of modeling admits of solving for cyclic states in polynomial complexity, for example by the Gauß-algorithm.

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[1] This paper is part one of three contributions dealing with the finite field description of finite state automata.

[2] The feedback design for multivariate linear discrete systems in a frequency domain like framework is subject of the second part of three papers on the finite field description of finite state automata.

[3] The analysis of multilinear systems using Gröbner-bases over $\mathbb{F}_2$ is considered in the third contribution, whereas this paper rather puts the stress on the theoretical base and the modeling aspects.

SYNTHESIS OF STATE FEEDBACK FOR LINEAR AUTOMATA IN THE FINITE FIELD $\mathbb{F}_2$ [1]

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In the first paper of this series we motivate the description of discrete event systems via state space models in the finite field $\mathbb{F}_2$. It is shown that in general, multilinear state equations are obtained. Further on, the problem of determining the cyclic states is solved for the subclass of linear automata. In the paper on hand, linear automata described as linear discrete systems over the finite field $\mathbb{F}_2$ are under concern. The state equation is as follows [1]:

$$\mathbf{x}[k+1] \quad = \quad \mathbf{A}\mathbf{x}[k] + \mathbf{B}\mathbf{u}[k].$$

In this case, the matrix $\mathbf{A}$ is the system dynamics, $\mathbf{B}$ is the input matrix, $\mathbf{x}[k]$ is the current state and $\mathbf{x}[k+1]$ is the next state, whereby all vector and matrix entries are binary. The most important property of this class of systems is the cyclicity of states[2], which uniquely corresponds to the elementary divisor polynomials of the system dynamics and can be directly related to the smith normal form of $\mathbf{A}$ [1], which has been shown in the first paper of this series. Based on this knowledge the synthesis of linear state feedback for imposing properties on the controlled system (concerning the cyclicity of states) is performed. By imposing these properties, the elementary divisor polynomials of the closed loop dynamics are set. In the scope of continuous systems this problem usually is solved by performing the parametric approach [2]. By means of this approach the synthesis of linear state feedback for linear multivariate systems can be carried out easily. To this end a closed-loop system with specified eigenvalues is established and the remaining degrees of freedom are used for adjusting the eigenspaces of the closed-loop system. Dealing with discrete systems in $\mathbb{F}_2$ this approach would involve specifying the zeros of the elementary divisor polynomials and determining the desired eigenspaces of the closed-loop system. As this idea emerges to be inappropriate another method for synthesizing a linear state feedback has to be employed. For linear continuous systems the polynomial matrix method in the frequency domain is used to compute a state feedback for achieving specified eigenvalues of the closed loop system by solving a diophantine equation [3]. This method is adapted to linear discrete systems over $\mathbb{F}_2$. At first the *$\mathcal{A}$-Transform* is introduced for generating a frequency domain-like representation of the given linear automaton [1]. Next a transfer function is defined for the linear automaton and a right polynomial matrix fraction description of this transfer function is obtained. The denominator matrix of this polynomial matrix fraction contains the similarity invariants and thus the cyclic properties of the original linear system. Due to this the synthesis problem reduces to specifying similarity invariants of the denominator matrix in the *$\mathcal{A}$-Domain* and computing the appropriate state feedback. This can easily be done by first evaluating an algorithm suggested by Kučera [3] and then utilizing the structure of a special normal form, the so-called controllability normal form. The latter is a major advantage in contrast to the usual method of solving a diophantine equation. By means of these results an algorithm is developed for generating a linear state feedback which fits a given linear automaton with specified cyclicity properties. Additionally the structural constraints for linear state feedback given by the structure theorem of Rosenbrock [3] are fulfilled automatically by the presented construction algorithm.

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[2] This topic is treated in the first paper of this series.

CELLULAR AUTOMATON MODELING OF THE AUTOBAHN TRAFFIC IN NORTH RHINE-WESTPHALIA

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Efficient vehicular transport of persons and goods is of vital importance to any modern society. In densely populated areas the capacity of the road network is often to its limits and frequent traffic jams cause a significant economic damage. Moreover, in these areas, it is usually hardly possible or socially untenable to build more roads. An intelligent use of the resource 'traffic infrastructure' is therefore economically crucial. The German state North Rhine-Westphalia (NRW) is an example of such a densely populated area where the capacity of the road network is not able to satisfy the traffic demand during the rush-hours. Every day there are traffic jams on the autobahns in the Rhine-Ruhr region (Dortmund, Duisburg, Düsseldorf, Essen, etc.) and in the area around Cologne and Leverkusen. To make things even worse, the traffic demand is still growing. For this reason, new information systems and traffic management concepts are clearly needed.

In 1992 Nagel and Schreckenberg proposed a stochastic cellular automaton model of vehicular traffic, which was able to reproduce some empirically observed non-trivial traffic phenomena like spontaneous traffic jam formation. This publication captured the interest of the physicists community and ever since there has been a continuous progress in the development of cellular automata models of vehicular traffic. The most recent models are able to reproduce free flow, spontaneous jam formation, synchronized traffic, as well as meta-stability. However, these models have one major drawback. They were developed and tested on topologically simple road networks and the translation to large and topologically complex real road networks is non-trivial. In our contribution we describe a micro-simulator, which is able to simulate the traffic flow on the autobahn network in the largest German state, i.e., North Rhine-Westphalia. The paper is organized as follows.

In Section 1 we discuss the traffic data available for the simulator. They are provided by a central server from "Landesbetrieb Straßenbau NRW", which sends date from about 4,000 loop-detectors, installed on the autobahn, minute by minute.

In Section 2 the cellular automaton model of vehicular traffic we use is described in detail. It is basically the Nagel-Schreckenberg model with smaller cells (1.5 m instead of 7.5 m), asymmetric lane change rules, a *slow-to-start rule*, *anticipation*, and *brake lights*. With these extensions the cellular automaton traffic model is able to reproduce all empirically observed traffic states. Further, we use two classes of different vehicles, *cars* and *trucks*, where the trucks have a lower maximum velocity and different lane changing rules. A vehicle occupies $2-5$ consequent cells.

In Section 3 we discuss some details of the implementation and the software design. The simulator was written in the C++ programming language and we use the *Glut OpenGL* 3D-graphics library for the visualization of the simulation. Because of the size of the autobahn network and because the simulator has to perform in at least real-time and preferably in multiple real time the algorithms used by the simulator have to be efficient. A further important design parameter is, that because there is a continuous process in the development of traffic models, it has to be reasonably simple to renew the dynamics. We give a short notice on the data structures and algorithms we used and we explain why we decided to use them.

In Section 4 we present some additions to the dynamics, which are necessary when modeling the traffic in a large and complex real road network, inclusive the assimilation of the traffic data.

Finally, in Section 5 we present the web-page *http://www.autobahn.nrw.de*, where the simulated traffic state on the autobahn in NRW can be viewed by the public and is updated every minute.

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Computing Systems and Discrete (Event) Systems

MODELLING OF RESPONSE TIME OF DISTRIBUTED DATA INTENSIVE COMPUTING SYSTEMS

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The distributed computational systems and the distribution algorithms are thoroughly studied. In this paper we focus on data intensive distributed problems including of task distributions, network delay times, join of the part task results, and the effect of non-execution. We make a study on „one box“ systems, dedicated multi computer systems, in which the number of computers, and the capacity of computers are almost constant and non-dedicated systems, when the number, and the free capacity of computers are frequently variable. The solution time of the full task depends on number of complex parameters, the effects of different parameters are well observed by modeling the behavior of distributed data intensive supercomputing systems. We show a frame for managing of this problem.
The users of the computers appraise the suitability and goodness of the systems by means of the response time, including the correct replays of course. The aim of this paper is to examine the reduction of the response time. Correct replays from the systems are assumed.
The elaborating time of the answer is influenced by the following components:

- network-times, network-delay times
- task-distribution times, and integration times of part-task results
- algorithm-times (processor times, running times)
- data-access times (local data access)

We examine the “one-box” systems shortly, and the “multi-box” systems in detail. There are two main types of task-distributions for multi-box systems, for the dedicated multi-box systems, and for the non-dedicated multi-box systems with variable number of computers.
In the dedicated multi-box systems the number and the capacity of computers does not change during the execution of the task essentially.
In the non-dedicated multi-box systems the number and the free capacity of used computers may change during the execution of the task.
Further important question is the non-execution of part-tasks. We have studied the managing and the effect of the redistribution.

Importance of the simulation. The algorithms, the network-situations, the errors appearing are various. They depend on very much parameters. Number of these parameters contain random or probability elements. Exact description of the elements is a hopeless task, which results very complicated formulas which hide the essential components. The simulation of data-intensive distributed systems offers a good help to find the quite good distribution strategy. In the paper we give some simulations examples and results. The simulation-algorithms give a possibility to use more variables and functions for modeling of different problems: the changing of the number of computers, for the manipulations with free capacity of computers, modeling the data distributions and use of distributed data. It is true, that the capacity of networks keeps growing, but the quantity of data and the size of data-intensive projects will be growing too, thus we assume that finding of the good distributions will be important in the future too.

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COMPUTATIONAL AND NUMERICAL ASPECTS OF REPEATED RUMOURS

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The spread of rumours can be regarded as a specific spread of information or disinformation. The models used to explain the spread of rumours serve as a tool to improve our understanding of this social phenomenon. Of particular interest is the phenomenon that the proportion of the population who never hear a rumour is non-zero. This in turn leads to the question of the behaviour of rumours that are initiated a second time—repeated rumours. To illustrate the implications of this result in an age of mass communication, it is natural to consider the initiation of a rumour by means of television, radio, or the Internet (Frost [3]). A typical example occurs with public health warnings through mass media following a poisoned food scare. Such warnings need to be repeated to maximize awareness of the information in the population. The stochastic analysis of rumours was introduced by Daley and Kendall [2]. In earlier work, Rapoport [5] and Rapoport and Rebhun [6] developed several models for the diffusion of information during the period 1948–54, using a deterministic approach to rumour modelling based on epidemic modelling. Two rumour models (Daley and Kendall [2] and Maki and Thompson [4]) are regarded as classical models in the literature. These models considered a single initial *spreader* introducing a *rumour* into a closed population. The Daley–Kendall model is given in continuous time while the Maki–Thompson model is formulated in discrete time. The effect of varying the initial number of spreaders from unity has been investigated by Belen and Pearce [1]. The perhaps surprising result was discovered that even when the proportion of the initial population who are spreaders tends to unity, the proportion of the initial ignorants who never hear the rumour will never be zero. In this paper we extend the Maki–Thompson model to allow for the initiation of a rumour by multiple spreaders, and the repetition of a rumour process. We derive an expression and give a solution for the proportion of the population who never hear the rumour, for a repeated rumour. We formulate a deterministic model in continuous time with arbitrary non-zero initial conditions specifying the initial proportions (of the total population) of three subpopulations—spreaders, ignorants (those who have not heard the rumour) and stiflers (those who have heard the rumour but do not spread it). It is usually assumed that the rate of convergence, with increasing population size, to the asymptotic results predicted by the classical models is slow. By analysing the results of a numerical method for the solution of our model we are able to determine experimentally the range of population sizes for which the model can reliably be applied. As a particular example we observe that, when the proportion of initial ignorants is 0.99, the estimated error for the model is negligible when population size exceeds 258. Thus it appears that asymptotic results can yield good approximations for quite small population sizes.

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TIME-OPTIMAL SCHEDULING FOR HIGH THROUGHPUT SCREENING PROCESSES USING CYCLIC DISCRETE EVENT MODELS

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High Throughput Screening (HTS) plants are used for the analysis of chemical or biological substances, where, for a large number of sample batches, several operations have to be executed in the same specific time scheme. While progressing through these operations, each single batch may pass the same machine more than once. More than one batch will be present in the system at the same time. There are no buffers between the machines. Moreover, a batch may occupy two or more machines simultaneously when being transferred from one machine to another. Additionally, there will be upper time bounds ('due dates') stated by the user.
Determining the time-optimal sequence and event times for all operations of a problem of several hundreds of batches ('assay') is therefore a scheduling task which is quite different from known scheduling problems in other areas of application as, e.g., in chemical engineering [2] or for flexible manufacturing systems.
For several specialized HTS plants, a number of scheduling approaches with a variety of objectives exists, e.g. [1]. However, as development goes towards large flexible HTS plants, a general scheduling approach is needed which can be used independently of the specific combination of machines and transport devices.
In many cases, due to the specific nature of the substances to be screened, operating schemes have to be strictly cyclic: The batches follow upon each other with constant time offset, called *cycle time* T. An extract from such a strictly cyclic schedule is pictured as a Gantt chart in Fig. 1.
We show how a timed discrete event model can be formulated for such cyclic sequences and how the scheduling problem can be cast into a mixed integer linear optimization problem. Its solution leads to a schedule with maximum throughput, i.e. minimum cycle time, and therefore to minimum overall processing time ('makespan'). The approach is demonstrated by means of a basic example.
It has been shown that the proposed method is suitable to solve real-world problems as they arise for a modern, fully automated flexible HTS system. Globally optimal solutions have been found for assays with up to 150 resource allocations per batch using GAMS/CPLEX.

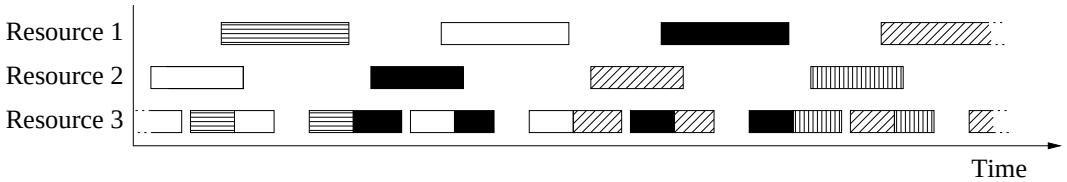

Fig. 1: Extract from cyclic schedule. Different patterns represent different batches.

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DEVELOPING MODELLING TOOLS FOR DISCRETE EVENT SYSTEMS IN THE DES/M ENVIRONMENT

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Technical systems that include complex physical dynamics as well as extensive discrete event control, require powerful modelling and simulation techniques. As the most adequate means for modelling hybrid physical systems, we advocate the use of object-oriented modelling languages such as Modelica. However, the discrete event models often require the use of dedicated graphical editors that can not be defined appropriately using Modelica. The purpose of the DES/M modelling environment [1] is to provide such editors for different discrete event formalisms and to translate discrete event models automatically into single Modelica components such that a discrete event controller can be integrated easily into Modelica models. This contribution presents the main concepts and techniques used in the DES/M environment to support problem-specific discrete event formalisms. This includes the automatic generation of graphical editors based on a syntax specification as well as the use of a model translation engine that accepts a high-level specification of a discrete event model to generate the Modelica code. Features such as sampling rates, concurrency and communication via shared variables can be considered and the Modelica code is such that frequent interruptions of the continuous integration due to periodical sampling is prevented.
The DoME tool allows to specify the syntax of graphical formalisms by means of a graphical meta-language that essentially corresponds to a class diagram. Based on this specification (meta-model) and appearance parameters the DoME tool generates a corresponding editor automatically. The meta-modelling approach of the DoME tool is restricted to the syntax and does not cover the semantics of a formalism. A practical way to establish the semantics of a new formalism is to use a formalism translation algorithm, that maps each proper model of the new formalism into a model of another formalism that has already a defined semantics. In the case of the DES/M environment, the language that represents the semantic foundation is Modelica. The translation of a discrete event model into a Modelica algorithm is a quite intricate task, because the developer has to consider numerical aspects as well. In order to simplify this task and to provide a way to use different formalisms in a hierarchical model, a model translation engine is used (fig. 1). This engine accepts high-level statements to build an internal formalism-neutral representation of discrete event models, and translates the complete representation automatically into a Modelica component. Thus, the formalism developer has merely to implement a translation algorithm that builds the intermediate representation of a model component. He can concentrate on the syntax and the input-output-behaviour of the formalism under development and needs not to consider knowledge on how the models will be represented in Modelica or how the interaction within hierarchical models will be implemented. The grey boxes in figure 1 depict the parts that have to be contributed by the formalism developer.

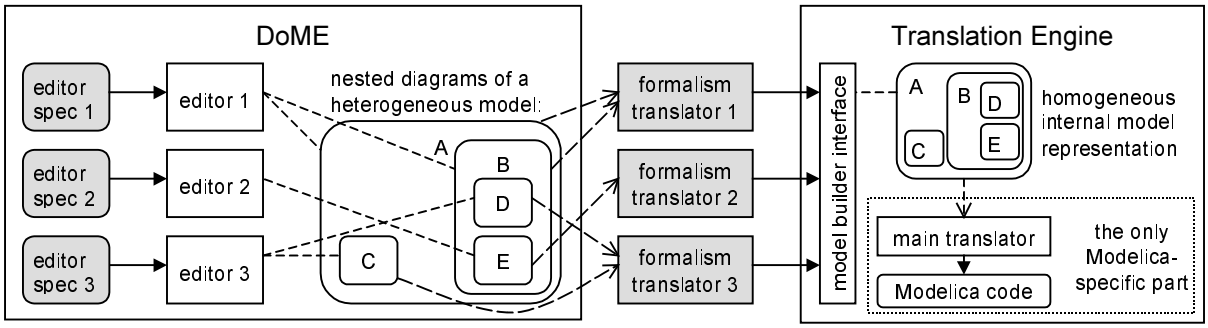

Figure1: The architecture of the DES/M environment

Keywords: Hybrid Systems, Modelling, Simulation, Modelica, Meta-Modelling, Formalism Translation

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Coupled Systems:
PDAE and SDAE Models in Technical Simulation

MODELING AND SIMULATION OF TRANSIENT NOISE IN CIRCUIT SIMULATION

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Simulation plays an important role for the development of integrated circuits, it helps to reduce the time necessary for the design as well as the production costs. A crucial point is the circuit simulation, this is the simulation of the chip on transistor level. Circuit simulation helps to verify the physical behavior of the circuit before producing test chips and allows for early corrections. Transient analysis is usually computed without taking noise effects into account. But due to the decreasing supply voltages and due to the decreasing size of the elements, this is no longer possible. The signal-to-noise ratio is getting so small that the noise effects have to be simulated, too. In most simulators this is done within the small-signal analysis, which means that only a linearization of the circuit is handled. Another approach is the non-linear frequency analysis for oscillatory circuits, which restricts the application to that special class of chips. To overcome this restriction, we will present a non-linear noise analysis combined with the transient simulation of the circuit. This analysis computes the so-called path of the noisy signals and allows the computation of the moments of the signals in a post-processing step.

An important prerequisite for a transient noise simulation is the proper modeling of the noise sources in the time domain. There are three main sources for noise in electronic circuits: Thermal noise, shot noise, and flicker noise. While the modeling of thermal and shot noise in the time domain is well understood and leads to white noise stochastic processes, the numerical treatment of flicker noise in the time domain requires some new approaches. Similar to the Brownian motion which (generalized) derivative is a white Gaussian process, we search for a stochastic process, which derivative has a spectrum of $1/f^{\beta}$, $0 < \beta < 1$. This process exists and is called *fractional Brownian motion*. For a numerical simulation of flicker noise in the time domain we have to construct random variables fulfilling the properties of the fractional Brownian motion. This task can be accomplished with the help of an appropriate covariance matrix.

From an engineer's point of view, the consideration of noise during the transient simulation means that appropriate noise sources are shunt in parallel to the ideal noiseless circuit elements. This gives an additional term in the underlying system of equations. For an efficient numerical treatment of the modified system, we need a new integration scheme specialized on the structure of the charge-oriented formulation of the equations. Some approaches for such schemes for stochastic differential-algebraic equations (SDAEs) will be presented. First results of transient noise simulation will be shown.

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Including semiconductor models in circuit simulation

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A model and index analysis of an electric circuit containing a semiconductor is presented. The modified nodal analysis of the electric circuit leads to a differential algebraic equation. This is coupled with a system of partial differential equations describing the semiconductor. The drift diffusion model, containing both elliptic and parabolic PDEs, is used to model the semiconductor.
The node potentials in the electric network supply boundary conditions for the electrostatic potential in the semiconductor. By considering the output current of the semiconductor into the electric network another coupling relation is obtained.
We will assume that the electric network without semiconductors is of index one. This assumption only depends on the topology of the network. Our goal is to examine the sensitivity of solutions of the coupled system with respect to time-dependent pertubations. For this the concept of the abstract differential algebraic system index is presented and applied.
Results are given on a simplified model of the semiconductors with charge carrier considered to be constant. Investigations in progress on the entire model is also presented.

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First order thermal PDAE models in electric circuit design.

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Already today, self-heating in integrated circuits is an important aspect, and the heat distribution affects the circuit's behavior. Especially SOI-based (Silicon-on-insulator) devices suffer from self-heating due to the technological built-in oxide-layer. This oxide separates body and substrate of the device electrically, which is wanted, but also thermally; thus it limits the heat flux out of the device. Therefore, to produce reliable designs, the heat evolution has to be taken into account and must be efficiently addressed by the circuit simulator.
To model the thermal effects within an integrated circuit, we present in this talk the accompanied thermal network model, which is based on distributed 1D and lumped 0D elements. On the one hand, this model includes that heat is stored and slowly conducted between elements (first order thermal interplay). And on the other hand, the applied approach of partially 1D description is guided by macro structures found in chip technology: here, the basic gates are lined up and separated by supplies and input shunts. This is in variance with the usual decoupled thermal networks, which describe only the local thermal evolution, insulated from each other.
The overall system for the heat evolution and the electric network consists of parabolic partial-differential equations (thermal part) and the well-known differential-algebraic network equations (electric part). We have summarized the total set of equations in the following Box.

electric network: (DAE-IVP) $\mathbf{A} = (\mathbf{A}_C, \mathbf{A}_G, \mathbf{A}_L, \mathbf{A}_I, \mathbf{A}_V)$

$$\mathbf{0} = \mathbf{A}_C \dot{\mathbf{q}}(\mathbf{A}_C^\top \mathbf{u}(t), \boxed{\mathbf{T}_C^{\mathrm{br}}}) + \mathbf{A}_G \mathbf{r}(\mathbf{A}_G^\top \mathbf{u}(t), \boxed{\mathbf{T}_G^{\mathrm{br}}, \mathbf{R}}) + \mathbf{A}_L \boldsymbol{\jmath}_L(t) + \mathbf{A}_I \boldsymbol{\imath}(t) + \mathbf{A}_V \boldsymbol{\jmath}_V(t)$$

$$\mathbf{0} = \dot{\boldsymbol{\phi}}(\boldsymbol{\jmath}_L(t), \boxed{\mathbf{T}_L^{\mathrm{br}}}) - \mathbf{A}_L^\top \mathbf{u}(t)$$

$$\mathbf{0} = \mathbf{A}_V^\top \mathbf{u}(t) - \mathbf{v}(t) \qquad \mathbf{x}(t_0) = (\mathbf{u}_0, \boldsymbol{\jmath}_{L,0}, \boldsymbol{\jmath}_{V,0})^\top \qquad \text{(IV)}$$

coupling interface: $(\boldsymbol{\jmath}_E = \boldsymbol{\jmath}_E(\mathbf{A}_G^\top \mathbf{u}, \boldsymbol{\jmath}_V))$

$$\left(\mathbf{E}_{\mathrm{tr}}(t)^\top,\ \mathbf{E}_{\mathrm{lp}}(t)^\top\right)^\top = \mathbf{E}(t) = \mathrm{diag}(\mathbf{K}\boldsymbol{\jmath}_E)\mathbf{A}_{\mathrm{tp}}^\top \mathbf{u}, \quad \mathbf{T}^{\mathrm{br}} = \mathbf{P}^\top \widehat{\mathbf{T}} \quad \mathbf{R} = \left(\int_0^1 \widetilde{\rho}_i(x, T_i(x,t))\,\mathrm{d}x\right)_1^m,$$

heat equation: (PDAE-BIVP) $\qquad i = 1, \ldots, m \qquad x \in \Omega = [0, 1]$

$$\text{(1D)} \quad M_i \dot{T}_i(x,t) = \nabla_x\left(\Lambda_i \nabla_x T_i(x,t)\right) - \gamma S_i \cdot (T_i(x,t) - T_{\mathrm{env}}) + \boxed{E_{\mathrm{tr},i}(t)} \cdot \frac{\widetilde{\rho}_i(x, T_i)}{R_i(t, T_i)}$$

$$\text{(0D)} \quad \widehat{\mathbf{M}}\dot{\widehat{\mathbf{T}}}(t) = (\mathbf{B}_{\mathrm{fac}}, -\mathbf{D}_{\mathrm{fac}}) \begin{pmatrix} \boldsymbol{\Lambda}(0)\nabla_x \mathbf{T}(0,t) \\ \boldsymbol{\Lambda}(1)\nabla_x \mathbf{T}(1,t) \end{pmatrix} - \gamma \widehat{\mathbf{S}}(\widehat{\mathbf{T}} - T_{\mathrm{env}} \mathbb{1}_k) + \mathbf{P} \boxed{\mathbf{E}_{\mathrm{lp}}(t)}$$

$$\text{(BC)} \quad \mathbf{T}(0,t) = \mathbf{B}_{\mathrm{fac}}^\top \widehat{\mathbf{T}}(t), \qquad \mathbf{T}(1,t) = \mathbf{D}_{\mathrm{fac}}^\top \widehat{\mathbf{T}}(t)$$

$$\text{(IC)} \quad \mathbf{T}(x,0) = T_{\mathrm{env}} \mathbb{1}_m$$

Furthermore, we discuss the coupling interface of the system, and establish physical properties such as positivity and strict passivity, showing soundness. Last, we outline a simulation technique, which takes into account the largely differing time scales: the multirate co-simulation.

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PRECONDITIONED SPLITTING AND OVERLAPPING TECHNIQUES IN MODULAR TIME INTEGRATION

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Complex technical systems are often composed of independently modeled subsystems. Examples are the interaction of pantograph and catenary in flexible multi body system simulation, or the impact of transmission lines effects on the functioning of a bipolar ring oscillator in refined electrical network modelling, where the compact subsystem is modeled by a differential-algebraic system, and the distributed subsystem by partial differential equations. In many simulation packages these PDE models are semi discretized in space by finite differences or elements, i.e. modelling and discretization are intertwined. At the end, one gets a differential-algebraic system (DAE) that is equivalent to an index-one system consisting of two DAE subsystems

$$\left.\begin{array}{rcl} \dot{y}_i(t) & = & f_i(y,z_i)\,, \\ 0 & = & h_i(y,z_i,u) \end{array}\right\} \quad (i=1,2)$$

that are coupled by algebraic equations

$$0 = g(y,z)\,.$$

This co-modelling ansatz is accomplished naturally by a co-simulation based on dynamic iteration exploiting the fine structure of the system, where the respective DAE submodels are solved iteratively. This approach allows for modular time integration that is very naturally based on the use of multi-method and multi-rate schemes.

If the modelling can be based on an Hamiltonian principle (as in the case of multi body systems and regular RLC networks), both subsystems define index-one systems with respect to y_i and z_i (Property A), and — together with the coupling equation — index-one systems with respect to y_i, z_i and w (Property B). In this case, stability and convergence of a dynamic iteration scheme, e.g. Picard, Jacobi, Gauss-Seidel iteration or any hybrid form, can be guaranteed iff two contractivity conditions hold for a stable error propagation of the algebraic component u. Stability and convergence can always be assured by low-level modifications such as changing the order of the subsystems or a matrix-valued preconditioning of the dynamic iteration [1].

In the case of charge/flux oriented formulation in circuit design, generally one of the properties A and/or B is violated, and stability may not be recovered by low-level modifications. However, stable alternatives can be constructed by using preconditioned splitting techniques that are based on topological network information [2].

More generally coupled index-1 DAE systems of the type

$$\left.\begin{array}{rcl} \dot{y}_i(t) & = & f_i(y_1,\ldots,y_r,z)\,, \\ 0 & = & g(y_1,\ldots,y_r,z) \end{array}\right\} \quad (i=1,\ldots,r)$$

allow for stable dynamic iteration schemes, if overlapping techniques are used. This approach will be motivated by examples from hydrodynamics ("alarm model Rhein") and multiphysical modelling (heat effects in SOI transistors).

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COUPLED SYSTEMS: PDAE AND SDAE MODELS IN TECHNICAL SIMULATION

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FINAL DISCUSSION

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The talks of the special session on *Coupled systems: PDAE and SDAE models in technical simulation* demonstrate the progress made within the consortium on *Numerical Simulation of Electrical Circuits in the Time Domain*. This network consists of three projects located at *Humboldt-Universität zu Berlin* and *Universität Karlsruhe*, which develop new mathematical methods for today's network analysis tools in cooperation with the semiconductor company Infineon Technologies. These projects are supported by the German Federal Ministry on Education and Research (Bundesministerium für Bildung und Forschung/BMBF) within the mathematics programme *New Mathematical Methods for Industry and Services*. The aim of this programme is to strengthen the use of mathematics in industry as the key technology of the 21st century.

The objective of the final discussion is twofold:

- to discuss future demands on modelling, numerical analysis and simulation of multi phenomenological systems and further applications in natural, engineering, life, social and economic science;
- to find out to what extent the experiences made within the German model of funding mathematics for industry may be exploited (or not) to better establish mathematics as the key technology on an European basis (e.g. within the scope of framework VI or subsequent EU research programmes);

Of course, the discussion will be open for any other topic associated to this special session.

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Financial and Economic Systems

TRADEOFFS OF AUSTRIAN BUDGETARY POLICIES: AN OPTIMUM CONTROL ANALYSIS

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Optimum control methods have been used in various studies to determine optimal intertemporal decisions for many problems in economics and operations research. For actual problems of policy-making at the macroeconomic level, an analytical approach has only limited relevance, because these problems are usually characterized by a great number of constraints as embodied in a model of medium or large size. Moreover, when optimal policies for macroeconomic decision problems have to be determined, uncertainty about policy effects has to be taken into account. Stochastic optimum control theory has not provided analytical solutions so far, except for very small problems. Therefore, numerical methods of dynamic optimization under uncertainty are the only means to solve problems of actual macroeconomic policy-making.

In this paper, we use an algorithm for determining optimal policies for nonlinear stochastic dynamic models to deal with the problem of designing optimal budgetary policies for Austria. This issue is of great political relevance, as can be seen from recent highly controversial policy debates in this country. We choose an approach of quantitative economic policy to determine numerically optimal budgetary policies for the next few years by minimizing an intertemporal objective function subject to the constraints given by an econometric model. This model, called FINPOL4, is a medium-size macroeconometric model for Austria, relating policy and exogenous variables to objective variables of Austrian economic policies. The objective function penalizes deviations of objective variables from their desired ("ideal") values. Exogenous variables of the model are forecast over the planning horizon, which is assumed to be 2002 to 2006, using time series methods. Optimal fiscal policies are calculated over this time horizon using the stochastic optimum control algorithm OPTCON. It is shown that optimal policies can improve on the performance of the Austrian economy as compared to a simulation using extrapolated values of budgetary policy variables. Moreover, quantitative assessments of trade-offs inherent in the Austrian economy are provided from a series of optimization experiments.

MULTIPERIOD PORTFOLIO SELECTION MODELS WITH TRANSACTION COSTS AND INITIAL HOLDINGS

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In this paper we extend Markowitz's portfolio selection model to multiperiod models which include proportional transaction costs in the presence of initial holdings for the investor. Our approach is new and is in the line of our previous papers. In order to reduce the amount of data (forecasts) from a series of experts a stationarity assumption is made. Our model will work well only if in the considered time horizon no great changes will be forecasted by the financial experts.
The standard portfolio model is one where an investor allocates his initial wealth among n risky assets. Assuming the assets returns are stochastic, Harry Markowitz (the 1990 Nobel laureate) in his pioneering work described a theory postulating that rational investors should select a portfolio from the set of all "feasible" portfolios which offers minimum risk for a given level of expected return and maximum expected return for a given level of risk. Since its introduction in the fifties, the model has dominated a great deal of the literature in portfolio analysis.
Pogue, in 1970, had extended Markowitz's portfolio selection model to include transaction costs, short sales, leverage policies and taxes.
The mathematical problem of optimally managing a portfolio of securities in the presence of transaction costs has received considerable research attention in recent years.
Practical portfolio investment problems under uncertainty are multiperiod problems. They can be modeled well as multiperiod stochastic programs. All the contributions, together with the progress in numerical methods, software and computer technologies gave an impulse to the development of large scale real life applications.The multiperiod models can handle the difficult problems of asset liability management and the strategic decision making under risk. For portfolio optimization problems, it is sufficient to deal with discrete time models since the investments are done at fixed time instants. The numerical optimization methods which need to be used to solve such problems seriously limit the level of detail in the uncertainty about future asset prices and returns which can be incorporated. There exist a large literature devoted to multiperiod portfolio optimization.
We study the problem of an investor who has some initial holdings and knows in a prescribed horizon of time the amount of payments (cash outflows) and the amount of cash inflows and the exact moments when these financial flows will take place. The time horizon is divided in m - 1 units which are called periods.
The investor has initial holdings in n assets. All the transaction are made only at the moments $t = 0,1,2,\ldots, m - 1$. The investor wants to withdraw at the initial moment $t = 0$ a sum of money equal to W_0. At moment $t = 1$ the investor wants to withdraw a sum of money equal to W_1, ..., at moment $t = m - 1$ the investor wants to withdraw a sum of money equal to W_{m-1}. In the case when some W_i is a nonnegative number we shall consider that the investor sells his assets in order to obtain an amount of cash equal to W_i. At period $t = 0$ the initial holdings of the investor are described by the vector $b = (b_1, b_2, ..., b_n)$, that is the investor had purchased before period $t = 0$ a quantity b_i of asset i, i=1,2.....,n. The aim of the investor is to find a two sequences of portfolios: $u_0, u_1, \ldots, u_{m-1}$ and $v_0, v_1, \ldots, v_{m-1}$ that minimize or maximize an objective map.
The sequence $u_0, u_1, \ldots, u_{m-1}$ represent the portfolios purchased by the investor at the moments $t = 0,1,2,\ldots, m - 1$. The sequence $v_0, v_1, \ldots, v_{m-1}$ represent the portfolios sold by the investor at the moments $t = 0,1,2,\ldots, m - 1$. In the portfolio selection models we study we suppose that the investor is rational, that is at the moments $t = 0,1,\ldots, m - 1$ when the investor is rebalancing his portfolio, he will not purchase assets which he will sell at the same moment.
In the paper are formulated three multiperiod portfolio selection models: The risk minimization model, the average return maximization model and the mean-variance model.
Two numerical examples are discussed for our risk minimization model.

A DYNAMIC MODEL OF PRODUCT POSITIONING AND ADAPTIVE AGENTS

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Whenever the decision about how to position a new product has to be taken it makes a difference whether the market is determined by horizontal or vertical differenciation. The first means that different attributes have different values from the viewpoint of the customers and the preferences are consistent. The latter means that choices depend on the individual taking the buying decision. [3] formulates an analytical model to show that in a two–player competition the cost–leader has an advantage in positioning her product. However, being confronted with data representing the customers wishes and/or the competitors decisions does not necesssarily mean a competitive advantage but it means the problem of correctly interpreting these data.
This paper elaborates on an agent–based simulation model featuring customers with equal purchasing power in a dynamic market of goods that may be substituted for each other. The customers always choose the product which best approximates their requirements. The price they are willing to pay for the product is fixed — in opposite to [3]. The supplying agents have only limited capacity to interpret their information about the competing suppliers or the customers. It is analyzed how adaptive agents, who use learning classifier systems (see [1]) to take their decisions and learn by using genetic algorithms, would position their products and how they react to a changing environment. Similar investigations were done by [2]. Four classes of suppliying agents occur in this market. Two of them consist of learning agents. The first group observes the positions (= needs) of the customers directly (we call them superior agents). The second group observes the positions of the suppliers and their profits (first class agents). The decisions for the next planning period are based on these observations. Additionally, there is a group of suppliers placing their products according to a "random walk" (second class agents), and another supplier who always chooses the position of the most successful seller of the previous period (imitating agent).
To compare these strategies on the demand side three behaviour patterns are taken into consideration: i) static, ii) cyclic, and iii) random walk. To allow accurate conclusions about the relation between customer behaviour and the success of a certain selling strategy, all the customers exhibit the same behaviour within one simulation. In the static scenario the imitating agent performs best. The suprerior and first class agents make a lower profit but are both at approximately the same level. The second class agents make almost no profit. If the demands change periodically, the sales of the imitating agent decline. This is due to the sudden change of the demands in every single time step. The imitating agent always moves to a position that was excellent in the previous period and will be excellent again in the following period. Finally, when the customers follow a random walk, the competitiveness is inverted. Both types of learning agents loose a big part of their market share and they even fall behind the second class agents, who were the losers in the other two scenarios. Again the level of superior and first class agents is nearly the same.

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AD-HOC RISK MANAGEMENT SYSTEM (ARMS) USING MULTIPLE REGRESSION WITH SCALED DUMMY VARIABLE (MRSDV) MODEL

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This paper proposes an ad-hoc risk management system (ARMS) by using a statistical method. The statistical model, referred to as Multiple Regression with Scaled Dummy Variable (MRSDV) is developed. MRSDV model focuses on the forecast and management of critical situations (e.g. critical network security breach, a terror event and the invest timing in stock market). A numerical simulation result is provided to verify the practicality and effectiveness of the proposed method. The MRSDV process is illustrated in Figure 1. The theoretical foundation for MRSDV model using k-point scaling as its dummy variable can be expressed as follows.

$$y_{ij} = \sum_{i=1}^{m}\sum_{j=1}^{t} \alpha_i x_{1ij} + \sum_{i=1}^{n}\sum_{j=1}^{t} \beta_i x_{2ij} + \sum_{i=1}^{k}\sum_{j=1}^{t} \gamma_i x_{1ij} x_{2ij} + \varepsilon_{ij}, \qquad \text{----------} \quad (1)$$

where y_{ij} : risk function (response)

x_{1ij} : quantitative independent variable

x_{2ij} : qualitative independent variable

α_i : coefficient of quantitative independent variable

β_i : coefficient of qualitative independent variable

γ_i : coefficient of product of quantitative and qualitative variable.

ε_{ij} : error term

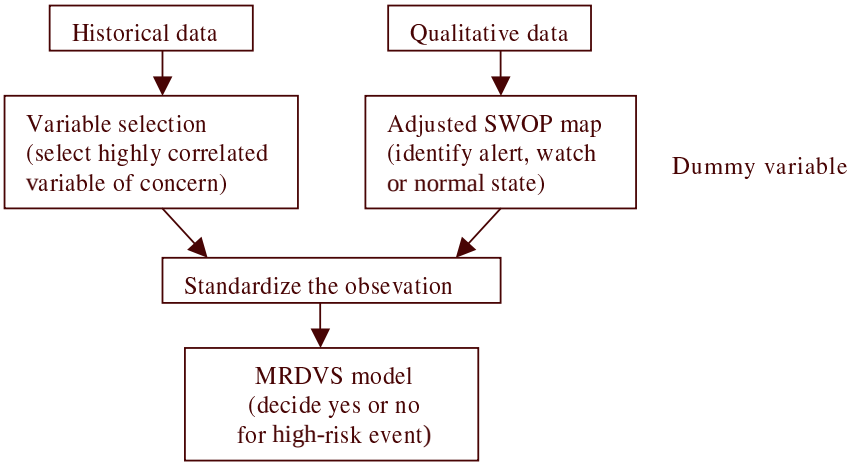

Figure 1 Procedure of MRSDV model.

The key advantage of MRSDV model is that it is practical to predict a high-risk event by using not only historical data but also the knowledge and intelligence of experts in field. The modelling effort also shows, if we accumulate the related data, the parameter of MRSDV model can become stable. This indicates the proposed MRSDV model is a powerful tool to predict unforeseen events.

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Computer-aided design system of simulation business-process model

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In the article the system is described, that allows to design static and the dynamic - simulation models of business process.

The system of simulation is intended for support the design process of complex business model. The complex model allows to analyze the qualitative - quantitative parameters of the business process and can be used by different categories of users - both managers, and systems analysts (programmers).

The analysis and reorganization (optimization) are the main purpose of the business processes description (simulation). The simulation modeling has recommended itself as the powerful tool of the complex systems analysis. The relation between simulation models and models of processes consists in conversion possibility of the processes model in the deficient simulation model. The simulation model gives more greater information for the systems analysis. The results of such analysis can cause of processes model modification.

The model of business process should give the answers for the following questions:

1. What procedures (function, operation) are necessary for obtaining finite result?
2. What sequence of these procedures?
3. What mechanisms of control and handle exist in the base of construed business process?
4. Who fulfils process procedures?
5. What incoming documents / information used by each process procedure?
6. What kind of outgoing documents / information are generating by the process procedures?
7. What resources are necessary for execution of each process?
8. What documentation / conditions are regulates execution of the procedure?
9. What parameters are characterize execution of procedures and process as a whole?

The existing computer-aided design system of business processes simulation have the following lacks:

1. Its does not allow integration with the simulation modeling systems, that allows to analyze qualitative - quantitative model parameters of business process;
2. Its used difficult language for model description, which difficult to use by the managers and analyzers, for which these models are created.

The main concept of the system consists in the description of the technological process as chains of operations, and simulation of behavior of firm (workers, equipment, state of material resources) and external environment (oscillation of demand on production (orders); oscillations of delivering of material, financial and other resources).

The kernel of modeling system for the technological process simulation is realized on a base discrete-events simulation method.

The solution of the task «What if» is carried out by change static and/or dynamic model of business process.

There is a floppy user interface for adding rules to the system, which will be generating messages when value of variable using in model is changed.

The simulation system allows to estimate main efficiency metrics of the technological process: probability of technological process failures; valid delays in technological process chain; a brave rating; the cost price of a unit of production; a estimate cost-return time of technological process.

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Automatic Control

NONLINEAR CONTROLLER DESIGN BASED ON ALGORITHMIC PLANT DESCRIPTION

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During the last two decades, several new methods for nonlinear controller and observer design have been developed [1]. Implementations of these algorithms usually rely on computer algebra packages for symbolic computations. However, the use for highly complex or large scale systems is limited due to a burden of symbolic computations involved [2].
Modern systems are often modelled using languages such as MODELICA or VHDL-AMS. This implies that the resulting plant to be controlled is not given by explicit mathematical formulas but by algorithms that may contain loops and conditional statements. Symbolic computation is not well-suited for this kind of model.
Many concepts for controller design are based on differential geometry. Hence, the computation of the controller usually involves the computation of special higher order derivatives (e.g., Lie derivaties, see below). Symbolic computation of higher order derivaties has one serious drawback: The size of the expressions increases exponentially w.r.t. to the order. Moreover, small modifications of the model result in time-consuming recomputations. A way to circumvent this problem is the usage of *automatic differentiation* [3]. The functions to be derived must be availible as an algorithm in a programming language.
Several types of derivatives are used in nonlinear control. Consider a nonlinear input-affine system

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})u, \quad y = h(\mathbf{x}) \tag{1}$$

with smooth maps $\mathbf{f}, \mathbf{g} : \mathbb{R}^n \to \mathbb{R}^n$ and $h : \mathbb{R}^n \to \mathbb{R}$. The *Lie derivative* of h along $\mathbf{f}$ is defined by $L_\mathbf{f} h(\mathbf{x}) := h'(\mathbf{x})\mathbf{f}(\mathbf{x})$. Higher order Lie derivatives are given by $L_\mathbf{f}^k h(\mathbf{x}) := L_\mathbf{f}(L_\mathbf{f}^{k-1} h(\mathbf{x}))$ with $L_\mathbf{f}^0 h(\mathbf{x}) := h(\mathbf{x})$. The gradient of the Lie derivative $L_\mathbf{f}^k h(\mathbf{x})$ is denoted by $dL_\mathbf{f}^k h(\mathbf{x})$. The *Lie bracket* of two vector fields $\mathbf{f}$ and $\mathbf{g}$ is given by $[\mathbf{f},\mathbf{g}](\mathbf{x}) := \mathbf{g}'(\mathbf{x})\mathbf{f}(\mathbf{x}) - \mathbf{f}'(\mathbf{x})\mathbf{g}(\mathbf{x})$. Iterated Lie brackets $[\mathbf{f},[\mathbf{f},\ldots,[\mathbf{f},\mathbf{g}]\cdots]]$ can be written as $ad_\mathbf{f}^k \mathbf{g}(\mathbf{x}) := [\mathbf{f}, ad_\mathbf{f}^{k-1}\mathbf{g}](\mathbf{x})$ with $ad_\mathbf{f}^0 \mathbf{g}(\mathbf{x}) := \mathbf{g}(\mathbf{x})$. Beside other applications, these different types of derivatives are needed for the following tasks in control theory:

Controller design: If (1) is input output linearizable [1], the stabilizing control law has the form $u(\mathbf{x}) = (v - L_\mathbf{f}^n h(\mathbf{x}) - k_{n-1} L_\mathbf{f}^{n-1} h(\mathbf{x}) - \cdots - k_1 L_\mathbf{f} h(\mathbf{x}) - k_0 h(\mathbf{x}))/(L_\mathbf{g} L_\mathbf{f}^{n-1} h(\mathbf{x}))$ with coefficients $k_0, \ldots, k_{n-1} \in \mathbb{R}$ and the new input v.

High gain observer design: The observer design procedure requires the nonlinear observability matrix $Q(\mathbf{x}) = (dh(\mathbf{x})^T, dL_\mathbf{f} h(\mathbf{x})^T, \cdots, dL_\mathbf{f}^{n-1} h(\mathbf{x})^T)^T$.

Design of extended Luenberger observers for nonlinear systems: Let $\mathbf{v}(\mathbf{x})$ be the last column of the inverse observability matrix. The observer gain $\mathbf{l}(\mathbf{x})$ can be computed applying a generalization of Ackermann's formula, i.e., $\mathbf{l}(\mathbf{x}) = (p_0 ad_{-\mathbf{f}}^0 + p_1 ad_{-\mathbf{f}}^1 + \cdots + p_{n-1} ad_{-\mathbf{f}}^{n-1} + ad_{-\mathbf{f}}^n) \circ \mathbf{v}(\mathbf{x})$ with $p_0, \ldots, p_{n-1} \in \mathbb{R}$.

If the model of the plant (1) is given in terms of a modelling language, symbolic controller and observer design procedures are not suitable any more. The computation of Lie derivates and Lie brackets using automatic differentiation requires a completely new framework [4]. This new approach we be explained on an example. In the contribution, the author will give further insights on the impact of an algorithmic plant desciption on controller and observer design.

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PARAMETRIC PROCESS MODEL FOR CONTROLLER DESIGN

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Recently, relay feedback tests have received a great deal of attention in system identification. The basic idea of the method is to bring the system into conditions of permanent oscillation by means of a relay which replaces the controller in the autonomous closed loop. From the relay feedback test, the familiar ultimate gain and ultimate frequency are readily available. Using the well known describing function approach parameters of simple transfer function models of process plants can be estimated. Based on the concept of the dual-input describing function (DIDF), Shen et al.[1] proposed a biased relay feedback which can identify a process static gain and its critical point in a single relay test. However, it is well known that being an approximate method the describing function method can yield inaccurate results. Wang et al.[2] have suggested a multiple point identification method from a single standard relay test for stable processes and their method needs to specify the values of decay factor, time span of computations and the number of the frequency response points. Atherton and Majhi [3] have proposed a novel method for accurate estimation of plant model parameters using symmetrical and asymmetrical relay feedback tests. However, in their method of identification a nonlinear algebraic equation solver has to be used to solve the simultaneous equations. Asymmetrical relay test enables one to estimate more number of unknown parameters of a model transfer function. To obtain non-symmetric input and output waveforms for lower order models and consequent exact expressions for the waveforms, asymmetrical relay test is generally prefered. But such identification method is subjected to highly inaccurate results in the presence of static load disturbances. The paper presents a novel method for the estimation of parametric model of completely unknown processes for autotune purposes. From a single symmetrical relay feedback analysis a set of general expressions are presented for on-line process identification. Using these expressions the parameters of open loop stable first order plus time delay (FOPDT) transfer function models may be obtained from simple measurements made on the limit cycle output. It has been reported in literature that one needs to solve complex nonlinear equations to find accurate model parameters of a process dynamics if approximations and approximate methods are to be avoided. The main contribution of the paper is to overcome the problems associated with solving a set of nonlinear equations simultaneously. Because problems may arise in that convergence may take place to a false solution if poor initial estimates are used. The initial slope of the output signal after a zero crossing can be measured. This extra measurement addresses the problem effectively. Now one needs to solve a single nonlinear equation instead of the set of nonlinear equations. The method is suitable for the processes that can be characterized by the first order plus dead-time model. It has been observed from extensive simulation studies that the proposed identification method gives quite improved results.

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DESIGN OF STABLE SUGENO CONTROLLERS WITH CONCENTRIC CHARACTERISTIC REGIONS USING SPHERICAL COORDINATES

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Whereas fuzzy control applications are widespread in most engineering fields, the stability and performance analysis of fuzzy controlled systems is still an open issue. In the case of Mamdani controllers with singleton consequents, called Sugeno controllers the state space can be partitioned in a number of regions where the control is bounded by affine-state controllers which parameters are regionwise valued and depend on the singleton values. Several methods allow to check the stability of nonlinear or piecewise linear systems combined with Sugeno controllers, generally consiting of finding a common quadratic Lyapunov function. One way of reducing the conservativeness of the solution is to relax the condition requiring the continuity of the Lyapunov function if the energy decreases when the trajectory moves from a cell into another. A main problem is the rather complex design procedure of Lyapunov functions and local domains. Whereas the fuzzy partition of the state space is polyhedral in general, a Takagi-Sugeno fuzzy structure which uses generalized spherical coordinates in the premise part is proposed in this paper, for which the characteristic regions are ellipsoidal or hollow ellipsoidal sectors. The rules take the form, in the state-space:

R_i : If ρ is ρ_i AND θ_1 is $\Theta_{i,1}$ AND ….. θ_n is $\Theta_{i,n-1}$ then $u = U_i$,

where $z = (\rho, \theta_1, ... \vartheta_{n-1})^T$ will correspond to a generalized spherical coordinates basis in the state-space.

It is assumed that the membership functions $\rho_i(.)$ are piecewise affine functions of the radius, and the membership functions of the angles $\Theta_{i,j}(.)$ are trigonometric.The regionwise nature of fuzzy systems/fuzzy control is put in evidence, and, in this case, it is shown that these systems may be bounded by piecewise affine systems/controllers. The shape of membership functions might be quite important to find the hard bounds. Modelling with spherical coordinates allows the regions to be (possibly hollow) sectors of ellipsoids; the model is control-oriented, since the boundaries of domains can be seen as an equipotential of a quadratic Lyapunov function. The controller model is closely linked to the TS model, with a regionwise constant set of parameters in the same regions. As a result, the design of discontinuous Lyapunov functions together with appropriate embedded sets will allow to derive relaxed stability conditions for a TS system with a corresponding Sugeno controller, which can be put under the form of a set of Linear Matrix Inequalities (LMIs) and relaxes the general stability condition.

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ALGEBRAIC MODELING OF LINEAR TIME-VARIANT SYSTEMS

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In this paper a new algebraic representation of linear time-variant dynamic systems is developed. It is shown that Walsh functions can be used to provide such a representation up to any desired precision.

Walsh functions have been widely used in different fields of system theorie. For example, Walsh functions have been applied in the modeling, analysis and time-domain synthesis of linear systems [1] and based upon Walsh functions in [3] an algebraic representation of linear time-invariant systems is presented. A comprehensive overview of the application of Walsh functions can be found in [2].

Walsh functions have been first introduced by Walsh [4]. They form a complete orthonormal set of rectangular waves in [0,1). Therefore, every function $f(t)$ which belongs to L^2, the set of quadratically integrable functions over [0,1) can be expanded formally in a series of the form

$$f(t) = \sum_{i=0}^{\infty} \hat{f}_i \cdot \mathrm{wal}_i(t) \tag{1}$$

where $\mathrm{wal}_i(t)$ is the i-th Walsh function and the constants $\hat{f}_i$ form the *sequency spectrum* of $f(t)$. It can be shown, that the series (1) converges uniformly. Thus, with $N = 2^m$ the truncated sum

$$f_{app}(t) = \sum_{i=0}^{N-1} \hat{f}_i \cdot \mathrm{wal}_i(t) \tag{2}$$

gives an approximation $f_{app}(t)$ of $f(t)$ with minimum integral square error. Another quite interesting feature of the Walsh transform $\mathcal{W}$ which will be extensively used in the paper is the existence of the so-called dyadic convolution theorem $\mathcal{W}\{f(t)\cdot g(t)\} = \hat{f} \circledast \hat{g}$ where $\circledast$ denotes dyadic multiplication of the corresponding sequency spectra. In the Walsh space S_N which consists of 2^m Walsh functions the finite sequency spectrum $\hat{\mathbf{f}}^T = [\hat{f}_0, \ldots, \hat{f}_{N-1}]$ of the stairstep function $\overline{\mathbf{f}}^T = [\overline{f}_0, \ldots, \overline{f}_{N-1}]$ can be calculated by means of the discrete Walsh transform $\hat{\mathbf{f}} = 1/N\, \mathbf{W}\, \overline{\mathbf{f}}$ where $\mathbf{W} = \mathbf{W}^T$, $\mathbf{W}^{-1} = 1/N\, \mathbf{W}$ is the symmetric, orthogonal *Walsh transformation matrix* and $\overline{f}_i = N \int_{i/N}^{(i+1)/N} f(t)\, dt$.

Based upon the Walsh transformation of linear time-variant dynamic systems an algebraic representation $\overline{\tilde{\mathbf{y}}} = \tilde{\mathbf{G}}\, \overline{\tilde{\mathbf{u}}}$ of such systems can be obtained, where the matrix $\tilde{\mathbf{G}}$ has a very special lower block triangular structure with the diagonal elements $\tilde{\mathbf{G}}_{ii}$ being the 'frozen' transfer function $\mathbf{G}(\tau_i, s_i)$ of the linear time-variant system evaluated at the N special points $s_i = 2\alpha i$ on the real axis of the complex plane and $\overline{\tilde{\mathbf{u}}}, \overline{\tilde{\mathbf{y}}}$ are the stairstep functions of the input respectively the output of the system over the transformed time interval $\tau = 1 - e^{-\alpha t} \in [0, 1)$.

Using this result new algebraic procedures for simulation, identifikation and controller design for linear time-variant systems can be developed. This is illustrated by the design of a time-variant PI-controller for a 6th-order linear time-variant multivariable system. To that purpose first the desired closed loop behaviour is specified in the shape of a linear time-invariant decoupled system and the time-variant controller parameters can then be determined from a simple set of linear equations.

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Closing loops: a unified view from control to information science

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In a previous work (1,2) a system-theoretic modeling approach is introduced, dealing with a special situation-operator modeling kernel (calculus), called (SOM). This modeling approach combines classical ideas of the situation and event calculus, and leads to a uniform and homogenous modeling approach describing human learning, planning and acting.
Understanding the human interaction with an outerside world as the complex feedback of a 'human controller' with the 'world to be controled', differences to classical (technical) control approaches appear. Classical technical control approaches consist of fix input-output relations, called controller, uses (usually) continous scalar physical values. The control design is done in advance with the background of a known control goal. On the other side the human learning and interaction capabilities are extremely flexible, but not fast. Changing environments (and control goals) can be understand, new connections can be setted, also algorithm-like strategies. The 'input-output' relation can be changed immediately.
After a short introduction into the Situation-Operator Modeling technique as background, the contribution deals with the classification of the distinctions between algorithms (and human control) on one hands side and classical control on the other. The classification also shows that between both, a lot of other known realizations (or from the point of view of the flexible human 'control': restrictions) exists, whereby the well known classical technical approach appears as the simpliest one (or from the point of view of the flexible human 'control': the version with the most restrictions). The items of the classifications will be clearly defined and detailed illustrated in the contribution with the examples of PID-control, Optimal control, Algorithms, Human Interaction, and Intelligent Systems. All examples spans a wide area for new types of technical realizations.
The goal of the contribution is the unified view to control from classical control approaches to approaches from information-science like SOM-approach (3). This gives - beside the academic scheme - the view to the next steps of improving automatic control algorithms. Based on microcontrollers, databases and intelligent datapreprocessing some 'human control' qualities like learning and flexible response abilities and situation control can be imitated by technical realizations.

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AN APPROACH TO CLOSED-LOOP SYSTEM DESIGN AND SENSITIVITY ANALYSIS BASED ON S-PLANE GEOMETRY

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.Single-input single-output closed-loop systems normally require some form of cascade compensator or controller to meet a given set of steady-state and transient performance requirements. This paper is concerned with an approach to the analysis and design of closed-loop systems that is based upon s-plane geometry and provides a very straightforward solution. This avoids the iterative processes normally associated with design based on frequency-domain or root locus design methods. The approach is applicable to single or multi-stage phase-lead or phase-lag cascade compensators and to three-term controllers involving proportional, integral and derivative elements. The approach represents an extension of methods that have been applied previously to simple cascade compensator design [2].

For a given set of performance requirements, expressed in terms of the gain factor needed to meet the steady state specifications and the location of the dominant closed-loop pole (or poles in the case of a specification involving a dominant complex pole pair), the approach provides the possibility of obtaining an exact solution. If the specification cannot be satisfied with the chosen form of controller, the method can provide an indication of the changes in the controller structure needed to make a design possible.

One of the fundamental problems associated with the interpretation of a system model having a predetermined structure (such as a closed-loop control system) is that of finding the particular parameters that have the greatest influence on the overall system performance. A necessary part of the controller design procedure is therefore determination of the sensitivities of the closed-loop pole positions to system parameter variations. One obvious solution is to carry out repeated analysis or perform simulation runs for each set of parameters but this often provides limited insight and is a tedious process. Other methods of parameter sensitivity analysis can provide an alternative and rather more efficient approach to this problem [3].

In the case of linear feedback systems, where the design procedures seek to predict closed-loop behaviour from open-loop system information, parameter sensitivities should also be determined from the open-loop characteristics. The effects of errors or uncertainties in parameter values can then be assessed as part of the design process. The approach to sensitivity analysis used in this paper [1] is also based on s-plane geometry and can thus be integrated within the processes for design of the cascade compensators or PID controllers.

Although geometric approaches to the analysis and design of closed-loop systems are not widely used at present, the availability of modern computational tools can assist greatly in terms of graphical interpretations and visualisation. It is believed that geometric approaches can provide useful design insight and can thus provide valuable teaching tools. The approach also allows students to be introduced to closed-loop system design and sensitivity concepts simultaneously and thus emphasises the need to integrate sensitivity analysis into the design process.

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APPLICATION OF ALGORITHM OF FORECASTING MODEL TO THE OPTIMAL CONTROL OF NUCLEAR REACTOR

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In this paper the problem of optimal control of a nuclear reactor is considered. It is required to increase the density of neutron flow from its given value at a given initial time to its given value at a given terminal time in such a way that the costs of control would be minimal. If one applies the standard objective function and the maximum principle this problem is reduced to a nonlinear two-point boundary value problem. Its solving encounters the computational difficulties and essentially depends on the choice of the initial approximation [4]. Besides, when the reactor parameters, such as the neutron life-time, are changing during the reactor work one has to repeat all calculations again and again.

In order to overcome these difficulties we apply an algorithm of forecasting model, the objective function being the function of generalized work [2,3]. In this case the boundary conditions for the terminal value of neutron flow are determined by the values of the weighted coefficients in the terminal part of objective function. It is essential that in this case there arises the Cauchy problem instead of the two boundary value problem. The corresponding numerical calculations result in the accurate terminal value of the neutron flow within the given limits for different values of the reactor parameters. But the values of the derivative of neutron flow at the terminal time turned out to be rather large (within 10-20 kW/s).

Further we generalize our approach. We apply the hierarchy with two functions of generalized work in the framework of the algorithm of step by step optimization [1]. This approach results not only in the accurate value of the neutron flow but also in the value of its derivative within the given limits (even less than 1 kW/s). The corresponding calculations show that application the algorithm of step by step optimization permits to provide more effective reaching the given value of the neutron flow density.

The quantities of calculations in the both cases (the simplified version of the algorithm of step by step optimization with the forecasting model and the algorithm with the objective function of generalized work) are of the same order.

It is shown that the considered algorithms are stable with respect to the changing of the neutron life-time during the reactor work.

Comparison the obtained results of modeling with the results obtained by the other methods with the Boltz objective function shows the high effectiveness of the algorithm of optimal control with the forecasting. Besides, the latter permits to find the optimal control in the case when the reactor parameters are changing during the reactor work.

The algorithm of forecasting model, the objective function being the function of generalized work, is the most effective approach to the description of the complex nonlinear systems and often it is a single optimal control which is formed in the real time. Moreover it is shown that this approach is also effective when the system parameters are changing.

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Bond Graph Modelling

FORCE AS FLOW OF MOMENTUM AND THE FORCE-FLOW ANALOGY OF BONDGRAPHS

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In a normal Bondgraph (BG), one uses the force-effort or direct analogy, with force as effort and velocity as flow. This is for rectilinear mechanics, while for rotary mechanics one has torque and rotation frequency. For the so called force-flow or inverse analogy, force is taken as flow and velocity as effort, also called Firestone analogy. It simply a permutation of effort and flow. These also and and pseudo BG are discussed and illustrated on the example of entropy conduction and heat conduction.

The direct analogy is generally used, but the inverse analogy has theoretical advantages: Force is considered as flow of momentum and all efforts become across variable with all flow as through variables. This facilitates formulation of mechanical BG and lead directly to another tool of systems analysis, the Linear Graphs. Furthermore. In the inverse analogy the flow of momentum is emphasized

Power handling in the oneports, twoports and multiports can be shown on a portality table, with the number of ports as X-axis and the properties of power handling on the Y-axis. By changing analogies, only some elements change place therein. For mechanical BG, in the inverse analogy all efforts are across variables and all flow through variables, which leads to a simplification of writing mechanical BG. Also another tool of Systems Engineering, the Linear Graphs can be applied. Here force is considered as flow of momentum. This underlines the importance of momentum, which is quantified in quantum mechanics and which simplifies the formulation of Newton's laws. A mechanics with the flow of momentum gives interesting results.

I have discussed these questions with Henry Paynter and we agreed, that mathematically it makes no difference which analogy is used. Intuitively, the inverse analogy is contrary to the feeling of most BG'ers including me, but it has theoretical advantages. So it is good to know both analogies

Relations between two bond graph approaches to sensitivity analysis and to robustness study

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Recently Borutzky and Granda proposed to construct a so-called *incremental* bond graph from an initial bond graph with nominal parameters in order to determine unnormalised frequency domain sensitivities in symbolic form. At the same time Dauphin-Tanguy and Kam presented a bond graph approach that allows to set up a specific form of state equations in symbolic form used for robustness study of models with uncertain parameters. Both approaches aiming at different purposes have been developed independently. Nevertheless, this paper shows that they can be used to obtain each other's results under some reasonable weak assumptions. For illustration both approaches are applied to an example, which has been kept fairly small for didactic reasons.

Keywords: Parameter sensitivities, equations for robustness study, incremental bond graph, uncertainty bond graph.

The design of a control of a system starts from a model that has been deduced either from physical principles under some assumptions, or obtained by system identification. Such a model may take the form of a matrix of transfer functions or a set of Differential Algebraic Equations (DAEs) depending on the objectives of the design. In any case one should be aware of shortcomings due to uncertainties. These may be caused by external hazardous perturbations, or/and may be due to insufficient, or erroneous parameter identification, or to tolerances in the fabrication process. This paper addresses parameter uncertainties. Two complementary approaches have been known for a long time. The first one addresses the determination of sensitivities of state variables or of output variables with regard to parameter variations. The second one aims at a robust closed loop control that ensures stability and a required system behavior within acceptable tolerance boundaries in presence of external hazardous perturbations and parameter variations. Models used for these objectives are *linear* in general. For robustness study either the *canonical form* or the *standard interconnection form* of state equations is used. For large systems considerable computational effort may be necessary to construct both forms symbolically even if a software package for symbolic manipulation is used.

The bond graph methodology, particularly suited for physical systems modelling, analysis, and control of multidisciplinary systems enables to represent parameter variations explicitly in a so-called *incremental* bond graph that can be derived systematically from an initial bond graph with nominal parameters. From the incremental bond graph parameter sensitivities as well as equations for robustness study can be derived in a systematic manner.

In the bond graph literature several authors use a pseudo bond graph for the determination of parameter sensitivities, in which the variables associated with the bonds are not power variables but sensitivities of the effort and the flow with respect to a parameter. Contrary, Borutzky and Granda recently proposed to construct from the initial bond graph with nominal parameters an *incremental* bond graph for the *variations* of power variables caused by small parameter changes. On the other hand Dauphin-Tanguy and Kam proposed a so-called *uncertainty* bond graph for true power variables that allows to derive a form of state equations used for robustness study. A comparison of both graph approaches reveals that both do have certain features in common although they have been developed independently for a different purpose. This paper shows that under some reasonable assumptions posing no essential constraints the incremental bond graph approach also allows to determine first order approximations of equations for robustness study, while the uncertainty bond graph approach can also be used to determine parameter sensitivities. Both approaches are applicable to bond graphs with stores in derivative causality and with algebraic loops. For the sake of brevity and clarity of the presentation however both cases are excluded in this paper. Moreover, stores and resistors are assumed to be linear 1-port elements.

This paper is organized in the following manner. First both methods are recalled. Subsequently, we show that the two approaches can lead to each other's results under some reasonable assumptions. Eventually for illustration the two methods are applied to a small example for which the results can be checked by hand calculation keeping in mind that the major benefit of both methods is the *automatic* derivation of sensitivities and of state equations for robustness study in symbolic form for *large* systems.

Structural Controllability for Switching Systems Modelled by Bond Graph

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Key Words: switched systems, bond graph, infinite mode, structural controllability

Abstract

Switching devices are very common in several fields (diodes, relays, clutches, valves, …). Their changes of states can be either controlled or autonomous. Various researchers investigated this problem using the bond graph tool [Karnopp,83], [Asher, 89], [Dauphin-Tanguy, 93], [Buisson, 93], [Lorenz, 93], [Strömberg, 95], [Cellier, 95], [Mosterman, 97], [Cormerais, 98]. Two main approaches, the ideal and the non-ideal one, are recalled:

- In the non-ideal approach [Dauphin-Tanguy, 89], switches are modelled as resistive elements eventually associated with modulated transformer. The modulation is done using a boolean variable. The main advantage of such an approach is that it leads to a unique causal bond graph model, whatever the position the switches can have.
- In the ideal approach, each switch is modelled as a null source: effort source for a closed switch state, and flow source for an open one. The state may be discontinuous at commutation times. This approach is used in this work.

In the other hand, in order to obtain a more realistic model for the analysis of system properties, the concept of structural property has been introduced by Lin (1974). It is a property, which is true for almost all the values of the parameters. This framework is consistent with physical reality in the sense that system parameter values are never exactly known, with an exception for zero values that express the absence of interactions or connections. The elements of a structural matrix are fixed either at zero or at indeterminate values that are *assumed to be independent*. Hence it is desirable to investigate system properties that are determined by the system structure and not by the parameter numerical values. These systems are called "structured systems".

The bond graph approach is used for the analysis of structural property of linear multivariable time invariant models. In the proposed bond graph approach, the structural property concept has been used. Nevertheless, the hypothesis of independence of the structural matrix terms (commonly used in the structural property study for structured systems by the digraph approach) is not seated.

This work is an extension of the structural analysis of generalized systems modelled by bond graph [Rahmani 98], [Mouhri 99, 00]. Here we consider switching devices modelled by bond graph as a good special case of generalised systems. This paper is organized as follows: first section is devoted to the recall of some useful background about bond graph modelling of switching devices. This modelling is done using the structure junction equation and leads to an implicit model $E\dot{x}(t) = Ax(t) + Bu(t)$. In a second section, structural ranks of the *E-*, *A-*, and *B*-matrices are proposed using causal manipulations on the bond graph model. It allows the determination of the minimum number of input sources necessary for control and the optimisation of their positions to simplify state feedback control laws. In section 3, the impulse controllability is defined as the ability to control impulse modes that singular systems can exhibit. In a first time a procedure which allows an easy determination of impulse modes from a bond graph model is presented. This procedure is based on causal manipulations. In the last step of section 4, a graphical method for structural impulse controllability is proposed. Finally, section 5 gives a practical example

Bond Graph Approach to Build Reduced Order Observers in Linear Time Invariant Systems

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Effective control and monitoring of a process requires reliable and continuous real-time information on the state variables of the process. In practice, however, continuous, on-line state measurements are rarely available. State estimators (observers), which are deterministic or stochastic, and static or dynamic systems, serve the purpose of reconstructing the inaccessible but important state variables from other easily available measurements. The Kalman filter and the Luenberger observer were the first ones to be introduced in the 1970s. The present work concerns deterministic linear time invariant systems modelled by bond graphs and because of that, the observers are built based on the Luenberger's method.
From an algebraic point of view, the Luenberger's method (1966) considers an observable linear time invariant system modelled by the following state equation:

$$\begin{aligned} \dot{x} &= Ax + Bu \\ y &= Cx \end{aligned} \tag{1}$$

with: $A \in \Re^{n\times n}$, $B \in \Re^{n\times p}$, $C \in \Re^{m\times n}$, y regroups the output variables of the system.
This method for reduced order observers divides the state variables of the model into measurable variables and non-measurable variables. The measurable variables are the state variables that can be directly measured from a sensor or can be calculated directly from the measurement of the sensor. With this classification, the state equation of the system can be written as a function of the measurable (x_a) and non-measurable (x_b) variables:

$$\begin{aligned} \begin{bmatrix} \dot{x}_a \\ \dot{x}_b \end{bmatrix} &= \begin{bmatrix} A_{aa} & A_{ab} \\ A_{ba} & A_{bb} \end{bmatrix} \begin{bmatrix} x_a \\ x_b \end{bmatrix} + \begin{bmatrix} B_a \\ B_b \end{bmatrix} u \\ y &= \begin{bmatrix} C_a & C_b \end{bmatrix} \begin{bmatrix} x_a \\ x_b \end{bmatrix} \end{aligned} \tag{2}$$

Afterwards, with a linear transformation, the state equation can be written as a function of the output and the non-measurable state:

$$\begin{bmatrix} \dot{y} \\ \dot{x}_b \end{bmatrix} = \begin{bmatrix} \bar{A}_{aa} & \bar{A}_{ab} \\ \bar{A}_{ba} & \bar{A}_{bb} \end{bmatrix} \begin{bmatrix} y \\ x_b \end{bmatrix} + \begin{bmatrix} \bar{B}_a \\ \bar{B}_b \end{bmatrix} u \tag{3}$$

This representation needs to inverse the C_a matrix. Because of that, after the selection of x_a, the condition: rank(C_a) = m must be verified to guarantee the existence of C_a^{-1}.
The principal advantage of implementing a reduced order observer is that it will estimate only those state variables which cannot be directly measured, thus, the order of the model of the observer will be lower than the order of a complete order observer, and therefore the computational cost to estimate these variables is also lower.
In this paper, the method proposed is a procedure to build the reduced order observers directly from the bond graph model. It can be used in both cases, when the output depends on all state variables and when the output is related to one state variable; in the second case the procedure is simpler.
The bond graph implementation is based on the Luenberger's method for reduced order observers in linear system (Luenberger, 1966). Because of that, it is necessary for the bond graph model to be equivalent to equation (1). It means that in the bond graph model there are no causal loops between R-elements or derivative causalities that could generate an implicit state equation.
The use of bond graphs allows employing techniques of structural analysis to determine the observability of a model, which is a necessary condition for the construction of Luenberger's observers. In this paper, the verification of structural observability of the bond graph model is made with the technique proposed by Sueur and Dauphin-Tanguy (1991).
With respect to the condition of the rank of C_a, it is shown how to determine the invertibility of the C_a matrix directly from the bond graph model and from a structural point of view.
Rahmani et al.(1994) proposed a method to calculate the gain of a controller gain for pole placement directly from the bond graph model. In the present work an extension of this method is used to calculate the observer gain. Because of that, it is possible to calculate the gain with the knowledge of the causal cycles families in the bond graph of the observer. In this case the characteristic polynomial of the reduced observer ($P_{(\bar{A}bb-K\bar{A}ab)}(s)$) is selected and then the calculus of K is based on the polynomial coefficients.
The main objective of this paper is to give a graphical method that can be applied on a bond graph model directly to build the observers without the generation and manipulation of the state and output equations of the system.
As an application, one example with two outputs is studied here, where one of the measurements depends on all state variables.

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ON THE PEDAGOGICAL VIRTUES OF BONDGRAPHS AND LINEAR GRAPHS FOR PHYSICAL SYSTEM MODELLING

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The use of bondgraphs (BG) or linear graphs (LG) has become standard for constructing models of discrete physical systems, i.e. those consisting of components with a finite number of localized points through which physical interactions can occur. These two methods have developed following distinct historical trajectories and they tend to be applied in different contexts and by different groups of modellers. Although it is obvious that BG and LG are based on the same basic concept, a generalization of Kirchhoff's electrical network theory and representation of the topology of the interconnection pattern of multi-terminal components which may be from any physical domain, it is widely believed that there are some significant technical differences between the methods and that certain types of applications are more suited for a BG or LG model. This view is incorrect. It has, in fact, been shown that physical system models based either method have exact equivalents in the other method. Moreover, as a representation of topological information related to system structure there is no difference between a BG and a LG. In effect, there are no technical differences. The only level in which there are differences, and in this respect these are obvious enough, is in the visual representation of the system diagrams themselves, i.e. the starting point for model construction which serves as an aid for mathematical manipulation and equation generation. It is natural to consider whether these (superficial and mathematically irrelevant) differences may lead to some pragmatic advantage of one method over the other, particularly from the pedagogical standpoint. This paper examines the virtues of bondgraphs and linear graphs as tools for developing and understanding physical system models, drawing from extensive experience in undergraduate teaching and practical model construction for applications. BG or LG provide a simple means for systematic model development which exploits the interconnection structure of the system components, clearly separating this from the representation of the physical laws (constitutive equations) which define their behaviour (Figure 1). Three pedagogical virtues shared by BG and LG are attributable to this explicit use of combinatorial information and its clear separation of this from physical behaviour: (i) physical analogy; (ii) causality; and (iii) energy flow.

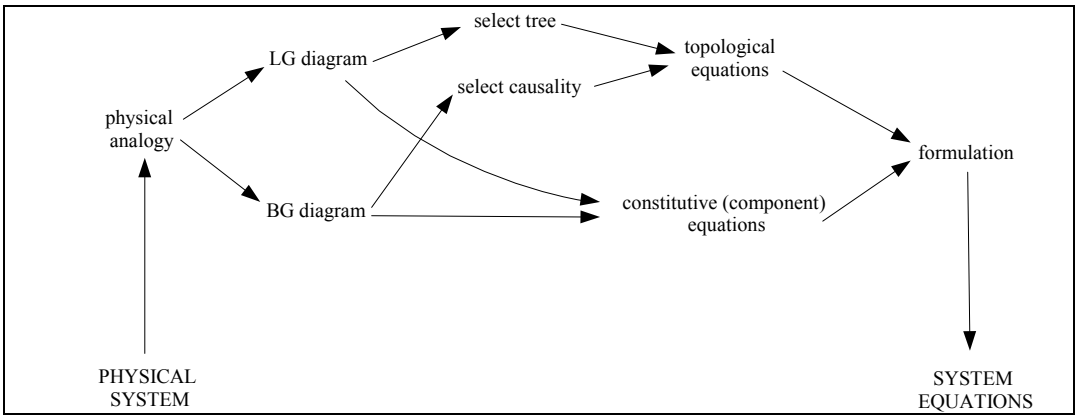

Figure 1. Derivation of physical system model equations using BG or LG methods. The sets of topological and component equations derived for the model are identical for parallel formulation methods. Alternative formulations common for LG, e.g. those which do not require a tree, are also available for BG, but not typically used.

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Physics of Computation

TREATMENT OF NON-EQUILIBRIUM MANY–BODY SYSTEMS: APPLICATION TO COHERENT OPTICAL PHENOMENA IN SEMICONDUCTOR MICROSTRUCTURES

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In the quantum regime, electron transition rates between different energy levels depend on the relative phase of competing coupling mechanisms. In such a a situation it is possible to control physical processes by an adjustment of relative phases between competing pathways. Quantum interference effects in form of constructive and destructive interference in the electronic wave function may serve as a fundamental principle for the operation of future mesoscopic electronic devices.[1] In semiconductors, first successful application of coherent control has been demonstrated in the last decade.[2, 3, 4]
Here we present a microscopic and non-phenomenological model for the interplay between coherent and incoherent charge carrier dynamics when exposed to external electromagnetic perturbations. It is based on a combination of non-equilibrium Green's function and density matrix techniques.[5, 6]
For the coupling of electrons to electromagnetic fields and an assessment of optical properties we have recently adopted two models: (a) the slowly-varying Maxwell equations and (b) a quantum description. The former is standard in quantum optics and allows a semi–classical treatment of external light fields, as well as the electromagnetic response of the sample.[7] The latter employs the photon picture and treats electron and photon dynamics on an equal footing. In contrast to the semi-classical approach, spontaneous emission is accounted for. This general approach has been applied to a number of studies in relation to coherent carrier dynamics and the feasibility of coherent control, including coherent manipulation of electron charge oscillations and terahertz radiation, optical absorption, optical gain, lasing without inversion, coherent control of optical phonon emission, and spin polarization. They have been based on a variety of excitation schemes and semiconductor structures.
In the talk we shall present numerical results for the self–consistent coherent and incoherent optical response of semiconductor microstructures and their coherent manipulation by external electromagnetic fields. In particular we address the possibility to coherently manipulate optical absorption and emission as a function of relative phase between a control and pump field in quantum–cascade–laser structures. The spectrally resolved induced electromagnetic field as obtained under various conditions will be presented. The role of open versus closed boundary conditions (current may flow through the system) and relevance to semiconductor implementations of quantum computers will be discussed.

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MATHEMATICAL MODELING FOR PHYSICALLY-COUPLED NANOSTRUCTURES

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The technology and physics of discrete nanoscale electronic components are reasonably well understood, but there exists a gap between device physics and nanoelectronic circuit integration. In this paper, we review our approach to the mathematical modelling of integrated circuits composed of Coulomb-coupled nanodevices and subcircuits of metal-contacted devices.[1] We assume that the Coulomb-coupled devices are far enough apart from each other that the overlap between their wave functions can be ignored. The internal electronic dynamics of the devices are described by quantum Markovian master equations, describing the dynamics of the devices as irreversible evolution of an open quantum system coupled to reservoirs. The electronic state of the devices is characterized by a finite-dimensional time-varying real vector. The state of the nuclei is characterized by classical state variables such as position and momenta. The Coulomb field generated by the device is described by the expectation value of the charge density approximated as multipole moments. Device-device couplings are determined by multipole interactions. In this way, the integrated circuit dynamics can be described by a set of coupled nonlinear differential equations. This set of mixed quantum-classical state equations leads us to the introduction of equivalent circuits. We conclude that integrated circuits composed of Coulomb-coupled and metal-contacted nanodevices do have circuit representations, thus circuit theory can be applied[2] to build device models, to simulate and to design nanoelectronic integrated circuits.

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Tools for Electronic Structure Computation

New Algorithmic Tools for Electronic Structure Computations

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Many mathematical models used in quantum mechanical computations, e.g., electronic structure computations for optical spectra (absorption and emission spectra), x-ray emission and diffraction, vibrational mode and rotational mode in molecules, tribology at electronic level, and material design, are built around the time-independent Schroedinger equation. Several interesting and challenging matrix problems result from various approaches for solving this PDE. Typically, no exact solutions are required, but some lower accuracy level which is defined by an application dependent accuracy parameter τ suffices.

Nonlinear Eigenvalue Problems. One approach for solving this equation involves a basis expansion of the unknown solution. A finite basis set is chosen and the original PDE problem is transformed into a nonlinear finite-dimensional matrix eigenvalue problem (for example, the Hartree-Fock equations). This nonlinear eigenvalue problem is often solved via a fixed-point iteration approach (called the Self-Consistent Field (SCF) method in quantum chemistry), which requires the solution of a linear real symmetric eigenvalue problem in every iteration.

A number of efficient algorithms for solving real symmetric eigenvalue problems is available. Depending on the nature of the matrices and desired spectral information, some require tridiagonalization of the original matrix as a preprocessing step, while others directly exploit the matrix's sparsity. However, the transformation to tridiagonal form can be expensive with unfavorable data access patterns and data locality problems for modern deep hierarchical memory computers, while alternative methods which do not require tridiagonalization tend to have disadvantages if large portions of the spectrum have to be computed. In the context of the SCF method, the linear eigenproblems have special properties which need to be exploited in order to achieve maximum efficiency. Since each of them is the inner operation in an inner-outer iterative structure, the accuracy requirement for each linear problem, defined by the inner accuracy parameter ν, depends on the given (outer) accuracy parameter τ.

We will summarize and discuss the capabilities and limitations of a new set of algorithmic tools for efficiently solving the linear eigenvalue problems arising in the SCF method. It is based on two central ideas - detection and utilization of matrix structure as well as approximation. It is well suited for all applications where the matrices arising in the SCF method are sparse or "effectively" sparse, i.e., where they have a large percentage of zero or "effectively zero" (with respect to the given accuracy parameter) elements. Given a matrix A and the accuracy parameter ν, the tools can be applied in two phases which correspond to the two central ideas mentioned before: block tridiagonalization and approximation of the spectrum of a block tridiagonal matrix.

In the first phase, an attempt is made to determine a sufficiently close matrix which has favorable structural properties. In this context, the goal is to determine a *block tridiagonal matrix B* (a generalization of a band matrix), whose eigenvalues differ from the ones of A at most by ν. We will outline a block tridiagonalization method which comprises a sparsification strategy, sensitivity analysis of the effects of individual matrix entries on the spectrum, and a covering strategy for determining a block tridiagonal structure which contains all nonzero entries of a given sparse matrix. This method is of particular interest in all applications where the original matrix A is diagonally heavy or exhibits other structural properties, because then this method can often find a closely related narrow block tridiagonal matrix.

In the second phase, a recently developed block tridiagonal divide-and-conquer eigensolver is available for efficiently approximating selected eigenpairs of B. This eigensolver has several attractive properties which make it well suited for the linear eigenproblems arising in the SCF method: It allows for arbitrary accuracy levels and exhibits proportionally reduced runtimes for lower accuracy requirements while being highly competitive if large portions of the spectrum or even the full spectrum needs to be approximated. We will also discuss parallelization strategies for this eigensolver which are currently implemented.

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FAST DENSITY FUNCTIONAL CALCULATIONS

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During the last years density functional theory (DFT) has become a very efficient tool for electronic structure calculations. DFT methods are fast and their accuracy is comparable to sophisticated ab-initio methods for many properties. Such a DFT method is the Gaussian plane waves (GPW) method [1] that uses two types of basis functions: (1) Gaussian-type functions for the description of the Kohn-Sham orbitals and (2) plane waves as an auxiliary basis set to expand the electronic charge density in order to combine the merits of both types of basis functions. A new implementation of the GPW method is presented, called QUICKSTEP, which is developed in the framework of the CP2K project [2]. A program structure which allows for an efficient parallelization of the code was considered from the very beginning. The very first benchmark results are presented and discussed.

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A PORTABLE SHORT VECTOR VERSION OF FFTW

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This paper presents a portable short vector extension for the popular software library FFTW—a library for the computation of the fast Fourier transforms (FFTs). FFTW is a freely available portable FFT software-library that achieves top performance across a large number of platforms.
The discrete Fourier transform (DFT) plays a central role in the field of scientific computing. The structural complexity of fast algorithms for computing the DFT, i. e., FFT algorithms, led to complicated algorithms which make it a challenging task to map them to standard hardware efficiently and an even harder problem to exploit special processor features like short vector extensions satisfactorily. By introducing double-precision short vector SIMD extensions like Intel's SSE 2, this technology entered scientific computing. Conventional scalar codes become obsolete on machines featuring these extensions as such codes utilize only a fraction of the potential performance. But these extensions have strong implications on the development of algorithms as their efficient utilization is not straightforward.
FFTW was the first effort that uses special purpose compiler techniques in combination with hardware adaptation using the actual runtime as cost function to overcome the difficulties of developing software that delivers high performance across platforms. The newly developed extension to FFTW enables the utilization of short vector extensions like Intel's SSE and SSE 2 as well as Motorola's AltiVec within FFTW for any problem sizes and is transparently for the user. The method is independent of the machine's vector length. It utilizes the C language extensions provided by compiler vendors (intrinsic or built-in functions and data types) to access the short vector hardware from within the high-level language and thus avoiding assembly language programming.
Experimental results show good speed-up for arbitrary problem sizes and excellent speed-up for problem sizes of powers of two and for non-powers of two which are multiples of 16. The newly developed short vector version of FFTW compares favorably with the hand-tuned vendor library Intel MKL on IA-32 compatible machines (Intel Pentium III and 4, and AMD Athlon XP).

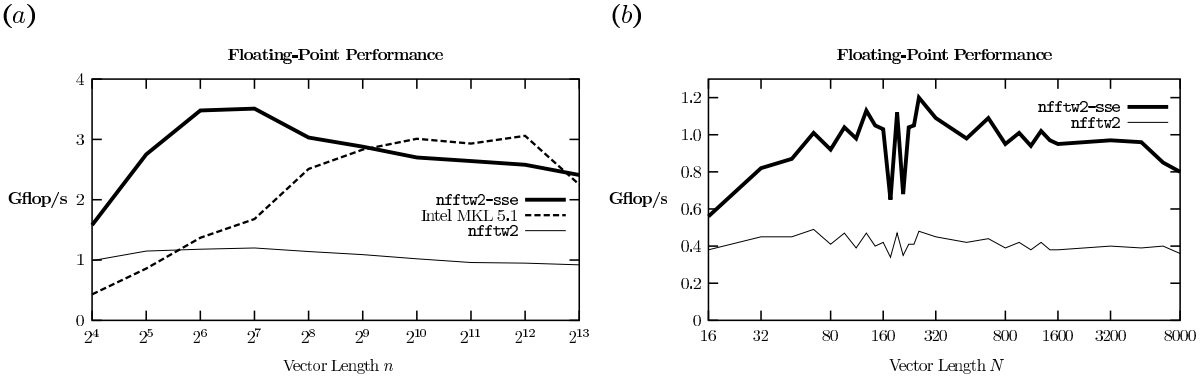

Figure 1: Performance results for (*a*) DFT_N, $N = 2^4, \ldots, 2^{13}$ on an Pentium 4 running at 1.8 GHz, and (*b*) DFT_N, $N = 16, \ldots, 8000$, $N = 16k$ on an Pentium III running at 650 MHz for single-precision and using SSE. The FFT programs compared are (*i*) the newly developed FFTW-SIMD (`nfftw2-sse`), (*ii*) the Intel MKL 3.5, and (*iii*) the original scalar FFTW version (`nfftw2`).

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An Improved Implementation of the Fast Multipole Method

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The Fast Multipole Method (FMM) [1, 2] calculates the potentials arise in various scientific applications. The direct method for evaluating these potentials requires $O(N^2)$ work regarding the number of particles. The Fast Multipole Method achieves linear scaling and enables the definition of error bounds.
The Fast Multipole Method consists of several steps. At first the particle coordinates are scaled so that all particles are enclosed by a box with coordinate ranges [0,1]x[0,1]x[0,1]. The parent box is devided in half along each Cartesian axis to yield a set of 8 smaller child boxes. The child boxes are subdivided again creating children of the children. The particles are sorted by box numbers using the radix sort algorithm [3] which scales linearly. The charges contained within each lowest level box are expanded in multipoles about the center of the box. The multipole expansions are translated to the center of the parent boxes. On each level the multipole expansions are transformed into local Taylor expansions. The parent's Taylor expansions are translated to the centers of the parent's children until the lowest level is reached. Each lowest level box contains a Taylor expansion representing the effects of all particles located in the far field region. The final step evaluates the interaction of all particles with the particles in the same box and in the boxes of the near field region.
Usually the Fast Multipole Method shows $O(L^4)$ scaling with regard to the length of the multipole expansions L. We have reduced the $O(L^4)$ scaling to $O(L^3)$ using the rotation based FMM [4]. For systems with more than a million of particles the Fast Multipole Method is not only substantially faster but also more accurate compared to the direct method. Calculations up to several billions of particles seem possible.

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Simulating the Performance of ScaLAPACK with Clue

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This paper describes CLUE, a tool for the accurate performance assessment and prediction of clusters of symmetric multiprocessors (SMPs). By using CLUE, the performance of different cluster configurations consisting of processing elements, memory, network etc. may be evaluated.
CLUE is based on MISS-PVM, which introduces an additional layer between the application program and the communication library, in this case the message passing library PVM. Messages sent over PVM are redirected into CLUE and drive the virtual simulation time. ALso, when entering the virtual layer, MISS-PVM measures the CPU time consumed since the last MISS-PVM call, which again increases the virtual time.
We have simulated the performance of the Cholesky factorization, the LU factorization, and the matrix-matrix multiplikation for 2000×2000 matrices on two different clusters. The Vienna Cluster was built and operated by the authors. It consists of five dual 350 MHz Pentium II systems ($p = 10$) with 256 MB main memory, 512 KB Level 2 cache and local 4.5 GB hard discs. The nodes are connected via a switched Fast Ethernet network (measured bandwidth: 12.5 MB/s).
The Aachen Cluster is a Siemens hpcLine PC cluster, consists of 16 dual processor boards equipped with 400 MHz Pentium II processors ($p = 32$), 512 KB Level 2 cache, 512 MB main memory and local 4 GB hard discs. The nodes communicate either via switched Fast Ethernet or SCI (Scalable Coherent Interface; measured bandwidth: 80 MB/s). The SCI network is configured as a two-dimensional torus. The network has been represented by a piecewise linear model.

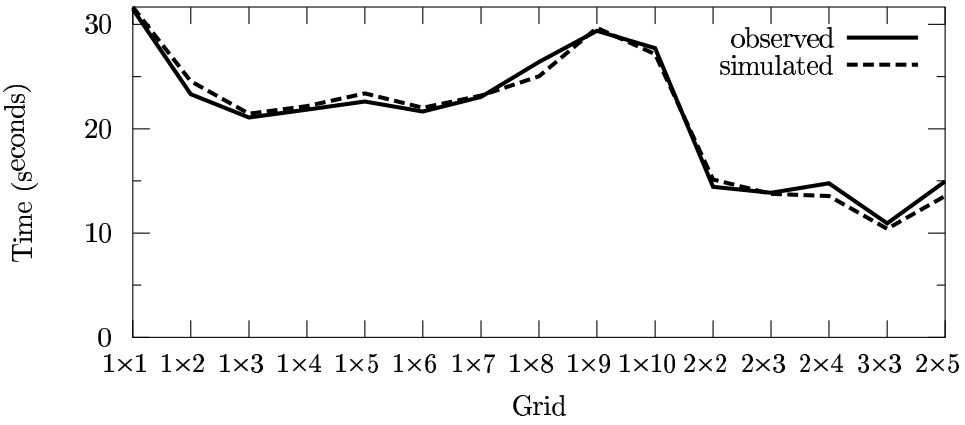

Figure 1: Cholesky factorization of a 2000×2000 matrix on the Vienna cluster. Blocksize 100.

As can be seen in Figure 1, the simulations show high qualitative and quantitative accuracy. The generated performance analysis may then guide potential cluster customers in their decision for one particular configuration.

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Combining Software Tools for System Engineering

SEMANTIC INTEGRATION OF MODELLING LANGUAGES BASED ON A REFERENCE LANGUAGE

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In computer-aided control system engineering, software tools are used to elaborate descriptions of dynamic systems for the purpose of simulation (e. g. of the environment) or specification and construction (e. g. of the controller). These system descriptions generally are called *models*. The tools therefore embody *modelling languages*, often with a graphical syntax (i.e. a model is a collection of related *diagrams*). The languages often are proprietary in the sense that they have no definition independent of a tool.

Like there is a language behind a modelling tool, there are formalisms behind a language. Several formalisms are well-known for the description of dynamic systems in different specializations, such as:

differential/algebraic equations for continuous variable systems
finite state machines for discrete event systems
imperative (i. e. state-based) programs

Their semantics are (or can be) defined mathematically. In order to achieve a useful language, one or more basic formalisms have to be combined with a collection of 'infrastructure' mechanisms, e.g. for hierarchical decomposition, abstraction and parameterization, or modularization. These additional formalisms also can be defined rigorously.

Every system description formalism defines a certain model of systems (also called a *system model*, which should rather be called a *meta-model* here in order to avoid confusion with the previously introduced individual models of individual systems). Many real-world systems are heterogeneous, i.e. they fall to components which do not fit very well to a single system meta-model but can be more naturally described by a combination of formalisms. Although some modelling languages reflect this, cases remain where a single existing language is not appropriate and a combination of languages (and tools) is desired.

In order to establish meaningful tool combinations, integrated meta-models for interfacing formalisms and languages are required. In other words, *semantic* integration is a presupposition of technical tool integration, which adds *syntactic* integration. On the other hand, semantic integration is preceded by methodical considerations providing for *pragmatic* integration.

For *semantic integration* of modelling languages we propose a *reference language* approach, consisting on the one hand of a reference language covering all relevant system description formalisms and a rich, orthogonal set of 'infrastructure' mechanisms, and on the other hand of mappings between (subsets of) existing modelling languages and (subsets of) the reference language. Thus, the linguistic interfaces can be defined on a profound mathematical basis and within a uniform syntactical framework.

A prototype of a tool integration based on the reference language concept has been developed to establish links based on model transformation between the commercial CASE tools MATLAB®/Simulink®, Statemate MAGNUM®, and Rodon®.

Model Integration by Co-Simulation applied to Hybrid Automotive Systems

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Improving system functionality within the automotive domain today is mainly done by increasing the portion of software in embedded systems. The way of developing this software is moving from traditional development strategies containing informal textual specification and manual coding techniques to a model-based engineering process beginning with requirements engineering and leading to automatic production code generation.

In order to advance this change of paradigm, the joint project STEP-X, which is a cooperation between the Volkswagen AG and the "Zentrum für Verkehr" at the Technical University of Braunschweig, was initiated. It aims to analyze existing methods, notations and tools in order to define a model based development process appropriate to automotive applications [1], integrating also testing and diagnostics.

One major constraint in STEP-X and for industrial applicability in general is to use standard CASE tools to ensure that project results can be used further on. It is important that commercial support and training are available. At the beginning of the project different CASE tools have been examined. One result has been that there is nothing available capable to provide all stages of the development process, starting with requirements management, finishing with automatic code generation and integrating test and diagnosis aspects as close as necessary. As indicated above, it is sometimes even in one certain stage demanded to use more than one CASE tool. Moreover, explicitly tool driven approaches turn out to be less advisable due to rapid changes within the tool market.

A possible solution is to couple different tools within (*horizontal* coupling) or among different stages of the development process (*vertical* coupling) by co-simulation. Concept and implementation approach of the Inter Tool Corporation (ITC) Framework is discussed [2], which has been developed at the Institute for Traffic Safety and Automation Engineering in Braunschweig (Germany). It is now commercially distributed, supported and advanced as the ExITE (Extessy Inter Tool Engineering) Toolbox, which is illustrated in a brief description. Finally, the application of co-simulation within the development process of the project STEP-X is described. Examples for the vertical and horizontal coupling are pointed out.

The application of tool coupling turns out to be a definite improvement, supporting the movement from classical manual development methods to a model based and CASE tool supported process. Especially in regard to the background of a heterogeneous and fast developing tool market, tool coupling is a possibility to reach a methodical tool independent development process instead of a tool driven procedure.

The main benefit of this approach is to become independent of CASE tool manufacturers by defining interfaces instead of tools. Coupling between different stages offers the possibility for meaningful simulation and analytical quality assurance in a very early stage. Co-simulation within one stage allows freedom for choosing methods and notations of the development process.

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Interval-Based Analysis in Embedded System Design

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Today's complex embedded systems integrate multiple hardware and software components, many of them re-used or provided as IP from different vendors. As a result of this growing complexity, an increasing amount of the overall design time is spent on system verification. Function verification is usually carried out on several levels of detail, starting from detailed model checking of small hardware and software blocks and ending with the abstract system-level functional analysis. Already verified functions can be added to the design without major effort.

The situation is different for the verification of non-functional system properties, e. g. timing and performance. There already exists a variety of formal timing analysis techniques for small sub-problems. But in contrast to the system function verification, they can not be simply composed into a system-level technique. In effect, timing and performance are currently only verified by performance simulation after system integration. This is because even functionally independent system parts may influence each others performance, since they compete for the shared resources. The known limitations of performance simulation such as incomplete coverage and corner case identification are aggravated since many of the design errors only result from system integration requiring detailed knowledge which is often not available to the integrator. In other words, reliable performance corner cases can be currently found for neither stage of the design process. This prevents the application of efficient modular techniques as known from function verification.

In summary, system performance verification is an unsolved problem. Many of the critical integration problems, such as buffer memory analysis and response time analysis could potentially be resolved by a formal global analysis if the known approaches to function verification could be extended to performance analysis without running into the problem of state space explosion. However, state space explosion would almost inevitably emerge when trying to analyze detailed system functionality, e. g. of a car, if this information were available at all.

We favor a fundamentally different approach which is based on explicitly introducing uncertainty into the system whenever we do not require behavioral details. We can do so, since the given performance constraints mostly allow a certain amount of uncertainty, too. A deadline, for instance, only constrains the maximum function execution time. Any earlier result delivery does not violate the constraint. Thus, a single upper bound can safely capture all possible timing behaviors of e. g. a task, even if this task is strongly input data dependent and has several different functional behaviors. The impact of resource sharing and task scheduling can be abstracted in a similar way. Only in distributed systems, the integration of several resources also requires lower bounds to be known due to the so-called scheduling anomalies. However, only upper and lower performance bounds of system components are sufficient to reliably and efficiently analyze the performance of todays complex embedded systems.

In this paper, we will analyze existing performance verification approaches and demonstrate the improvements of applying the proposed interval-based analysis in terms of efficiency and design comprehensibility. Then, we will successively derive a system-level performance analysis procedure. The key enabler is an interval-based representation at the interface between individual sub-problem techniques

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Models and Estimation of Waste Water Treatment

SYNTHESIS OF MODEL BASED OBSERVERS FOR ACTIVATED SLUDGE PROCESSES

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Abstract. This paper deals with the design of observers of unmeasured states for activated sludge processes. The synthesis is evaluated from the plant configuration proposed by the Benchmark of the European group COST 624, which is considered as a typical plant, and enables to point out their general relevance independently from process specificities. The observers presented in this paper are the most commonly used on real processes: an extended asymptotic observer and an extended Kalman filter. They are based on an accurate reduce order model from the very complex model proposed in the Benchmark. A discussion about the interest of each observer, as for instance the choice of the measured and estimated variables, the easiness to implement and their performances, is proposed and will help for the choice of the observer technique in a real plant.

REFINEMENT OF AN AEROBIC BIO-REACTOR MODEL

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The accepted model for standard batch operation of Sequencing Batch Reactors (SBR) used in the treatment of toxic wastewaters resulted insufficiently detailed for implementing optimal control strategies that require the estimation of substrate by using oxygen based observers. In such fed batch case, the substrate –the main control variable- is assumed to be non measurable, and thus must be estimated via oxygen measurements. The performance of such estimation depends in great deal on the fitness of the mathematical model used for the bio-reactor.

Three modifications are proposed, such that an adequate level of simplicity vs. performance compromise is achieved.

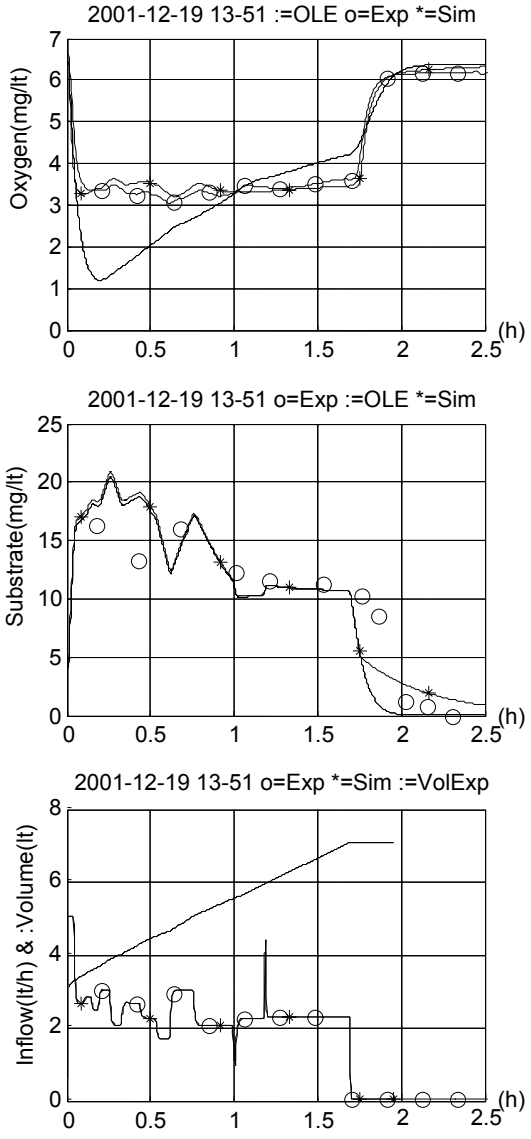
The oxygen dynamics is altered to depend on both the reactor volume level and its substrate concentration. For the first part, a simplified law for explaining the change of the "oxygen mass transportation coefficient" $K_l a$ as the reactor fills is proposed. This is especially critical when using optimal strategies that fill the reactor slowly when confronted with peak substrate concentrations in the influent. Such law proved to be usable in the working volume range for the test reactor, even for a non standard conic-cylindrical geometry.

For the second part, a lineal change law is proposed, assuming that the more substrate there is in the compound, the more effective is the oxygen transference from the air bubbles to the liquid medium.

The third modification proposed is the inclusion of an initial threshold for the "Specific biomass growth rate" *mu(S)*. This allows to somehow justify the fast changes in oxygen observed after substrate depletion when the reaction finishes.

These modifications were tested on simulation and also validated with experimental results.

The figure shows the experimental results (circles) vs. simulation results using the new model (continuous-star) and compared to the simulation results using the former model (dotted). Pay special attention to the Oxygen graph, where it can be seen that the simulated data using the refined model closely resembles the experimental data.



Isolability of Multi-leaks in a Pipeline

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Abstract. The automatic detection and location of multi-leaks in pipelines is a challenge for the process control and supervision engineering. Several schemes of leaks location based in the mathematical model of the ‡uid have been developed in the last decades by the safe process community. However all the approaches can produce false location leak if simultaneous leaks appear in the pipeline. This contribution discusses the detectability and isolability problem for two simultaneous leaks in a pipeline when only pressure and ‡ow rate are measured at the end of the line. In particular, it is shown that the leaks are detectable but the isolability problem is not feasible without considering the dynamic of the ‡uid if the leaks appears simultaneously. The analysis is made using physical relations of the ‡uid and showing that for any ‡ow rate loss in the pipeline, a unidenti…cable subset of leaks conditions is generated. Moreover, a new parameter de…ned as z_{eq} which characterizes the subset of undistinguishable subset of leaks is introduced. This new parameter allows to estimate leak region only in a imprecise way: if only a leak is present its location is estimated by the value z_{eq} and if two leaks of the subset appears simultaneously one can say that a leak is located to the left of point z_{eq} and the other to the right of it.

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Visual Prostheses

RETINAL PROTHESIS: ASSESSMENT OF THE QUALITY OF SEEING ACHIEVABLE BY SUBRETINAL ELECTRICAL STIMULATION

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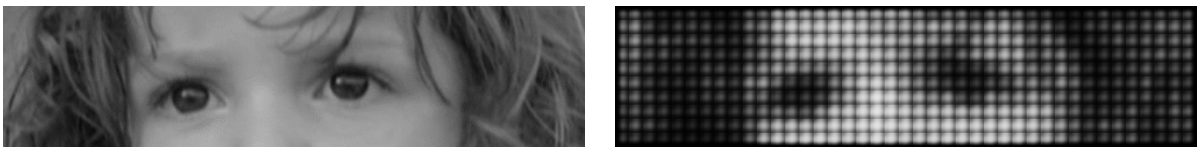
Electronic devices implanted into the retina of blind people suffering from photoreceptor degeneration are intended to restore vision by electrical stimulation of retinal neurons [1]. Currently, a subretinal device is under development for implantation between the pigment epithelial layer and the outer layer of the retina. It contains an array of micro photodiodes (MPD) and amplifiers to convert the local intensity distribution of the retinal image projected onto the array into a corresponding pattern of stimulating voltage levels [2]. Via a two-dimensional array of stimulation electrodes this encoded visual information is fed into the visual pathway by multisite excitation of the partially degenerated retinal network. To approach the question whether this kind of retinal stimulation is useful for vision we constructed a very simplified model of the retinal output. The model is based on the results of *in vitro* experiments with explanted retinas [3] and includes the functional properties of the 1st generation active subretinal implant. It neglects horizontal interactions of retinal neurons.

For approaching the retinal output produced by subretinally implanted MPD arrays we simulated the transformation of retinal images of natural and artificial scenes into static retinal activity patterns. Images were sampled into rectangular mosaics with 40 by 40 elements of size 70 x 70 µm². The differences between the average intensities of single mosaic elements and the fullfield average intensity were converted into discrete voltage levels for multifocal electrical stimulation. Focal stimulation produces a spatially confined retinal polarisation, that we described by a Gaussian-like spatial function. By linear summation of the activation profiles of all stimulation sites we obtained 2D retinal polarisation patterns. According to the tuning curves of single ganglion cells for focal electrical stimulation [3], we transformed this pattern into a static 2D activity pattern resembling the retinal output.

The simulated retinal activity pattern reproduces well-ordered distinguishable contrast and form features of retinal images that are almost independent from the absolute light intensity. Critical to the result is the lateral spreading of the focally injected charge that affects the width of the polarisation profile and the sensitivity of retinal columns to electrical stimulation. On the level of the retinal input, narrow profiles leads to separated foci whereas wide profiles lead to pixel fusion and local blurring, which decreases the content of spatial frequencies in the polarisation pattern.

Experiments in vivo have shown that activity evoked by subretinal electrical stimulation is projected retinotopically correct to the visual cortex. Therefore, we conclude that the well ordered spatial activation of degenerated retina is transformed into a coherent cortical activation that will be sufficient for useful visual perception in blind humans.



Simulation of the retinal output evoked by an subretinal implant (left: retinal image, right: evoked ganglion cell activity)

Supported by BMBF Grants 01IN502C (MPD-Array), 01KP0009 (Retina Implant)

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A modelling approach of the intra-orbital optic nerve stimulation

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Some types of total blindness, and mainly retinitis pigmentosa (RP), are characterized by the loss of photoreceptor cells of the retina while a significant number of ganglion cells and their axonal processes survive. This suggests the possibility to develop a visual prosthesis based on the direct electrical stimulation of these cells. A blind RP volunteer has been intra-cranially implanted with a self-sizing spiral cuff electrode around the optic nerve [3]. Electrical stimuli applied to the nerve allowed the perception of localized phosphenes in a safe and reproducible way.
Although previously successful, the intra-cranial implantation has several drawbacks, and an attempt to implant intra-orbitally a cuff electrode around the optic nerve is foreseen. The issue of whether or not to remove the dura mater at the implantation site is critical. Indeed, placing the cuff around the highly resistive dura layer could cause excessive activation thresholds and a very low selectivity. Besides, peeling off a segment of the dura is a technically complex and hazardous surgical operation.

A modelling approach can help to solve this dilemma. Several volume conductor models have been built, representing respectively : the cuff implanted over the pia mater; the cuff electrode placed directly around the dura mater; and the cuff over the pia mater after growing of connective tissue at the implantation site. The 3D electrical potential is then computed for these different geometries using a 2D Finite Elements approach coupled with a semi-analytical Fourier spectral decomposition to approximate the solution behavior in the azymuthal direction [2]. The resulting solution is then used to calculate the response of the optic nerve fibres to the stimulation. For this purpose, a classical myelinated membrane model has been adapted in order to fit optic nerve experimental data [1]. The influence on the simulation results of the conductivity of critical layers, such as the dura and the connective tissue, is carefully analyzed by comparing excitation thresholds and activation maps.

Simulation results show that optic nerve activation with a cuff electrode around the dura is possible. Depending on the effective value of the dura resistivity, the corresponding range of thresholds is between three to twelve times more important, for identical fibres, than the thresholds of the situation where the dura is removed. Nevertheless all calculated thresholds lie within the safety limits. In the case of a too highly resistive dura layer, selectivity could become critical. In case of a removed dura, if some connective tissue grows between the electrode cuff and the optic nerve, thresholds increase but remain limited, being still lower than when the dura is present.
To conclude, this modelling study tend to show that a visual prosthesis based upon an electrode cuff intra-orbitally implanted around the dura mater should be feasible. Experimental studies and mostly impedance measurements still need to be undertaken to confirm these assumptions, give useful data to refine the model, and ultimately determine the final implantation procedure

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MINIATURIZATION OF ELECTRODES TOWARDS SINGLE CELL STIMULATION IN NEURAL PROSTHESES -POTENTIALS AND LIMITATIONS

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Neural prostheses [1] use the principle of technical excitability of nerves by means of electrical stimulation and the feedback of bioelectrical signals to control technical devices in neurological rehabilitation to restore body functions. Cardiac and phrenic pacemakers, systems for deep brain stimulation in Parkinson's disease, and cochlea implants are the best known examples for neural prostheses. During the last decades, these implants have been fabricated with means of precision mechanics to obtain small and robust systems. Since microsystem technology paves the way to structure sizes in biological dimensions, new application scenarios for miniaturized neural implants that were unapproachable with means of precision mechanics seem to be feasible. The combination of microelectronic and micromechanic principles in the design and development of implants enables the possibility to integrate a high numbers of electrodes with stimulation circuitry on a single chip or in a highly integrated hybrid assembly. Flexible electrodes (Fig.1) and substrates [2] improve the structural biocompatibility of the implants from one-channel electrodes up to complex retina implant systems.

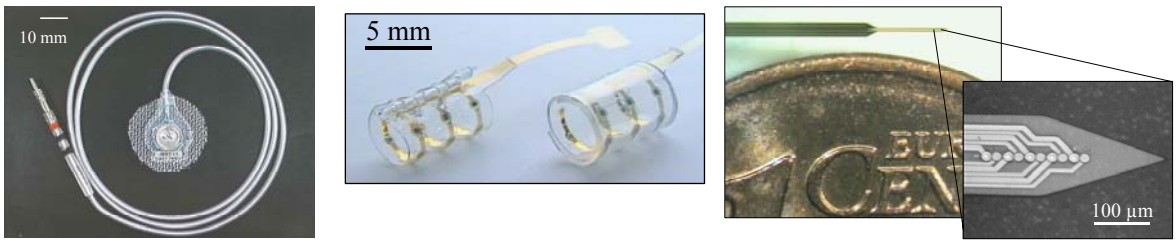

Fig. 1: Different steps of miniaturization of electrodes: single channel epimysial electrode (left), stimulation cuffs with micromachined electrode array (middle), brain microprobe (right).

Since the spatio-temporal interaction of multiple channel stimulation on complex biological tissue, e.g. the cochlea or the retina, cannot be foreseen, simulation of potential distribution in neural cell ensembles and nerves is mandatory for the design and optimisation of neural prostheses. This work has been done in several research groups for decades. Until now, the simulation starts on the level of nerve and tissue properties and decisions at which potential gradient or current density a nerve would be excited or which potential gradient might lead to refractory states of different nerve fibers. So far, the interface properties between the metal surface of the electrodes and the nervous tissue have not been taken into account but only point current or simplest geometries have been postulated.

Miniaturization down to the cellular level sounds very interesting but with the known materials from today the functionality of the electrodes might limit their size as well as physical limitations do. In this paper, models of the electrode-electrolyte interface that correspond to the electrochemical mechanism at the phase boundary are introduced. Different models of the phase boundary were validated from several electrode sizes. Aspects of electrode geometry and size are discussed as well as the influence of the current density and polarization effects at the interface. Ongoing work will focus on the modelling of the electrochemical properties of the electrode-electrolyte phase boundary as well as the electrode-tissue coupling. Micro- and Nanostructures of the electrode surface, nonlinear, current depending impedance of the electrode-electrolyte phase boundary as well as inhomogeneities due to protein adsorption or cell adhesion and cell proliferation on active surface.

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THE ELECTRICALLY STIMULATED RETINA: A SIMULATION STUDY

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Objectives. Based on a principle and technology already clinical routine with cochlear implants, retinal implants are supposed to enable blind people to see. Although patients with diseases like age-related macular degeneration or retinitis pigmentosa are blind, they posses functioning bipolar and ganglion cells, which relay retinal input to the brain. A combination of experimental work and computational modeling is necessary to clarify the complicated retinal functions.

Methods. In a two step procedure the excitation of electrically stimulated retinal cells is simulated: (i) the extracellular potential along the neural structure is computed (ii) the target cells are represented by compartment models. Membrane kinetics of the ganglion cells are evaluated with the Fohlmeister-Colman-Miller (FCM) model. Transmembrane voltages of the bipolar cells are calculated for constant membrane conductance.

Results. In retinal ganglion cells the axons are the most excitable structures when stimulated with short cathodic pulses from epiretinal electrodes, whereas the axonal endings are the hot spots in bipolar cells. Maximum induced membrane voltages strongly depend on neural geometry and orientation relative to the electric field. **Conclusions.** Bipolar cells in the retina are expected to respond with neurotransmitter release, before a spike is generated in the ganglion cells, even when bipolar cells are more distant to the electrode.

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INVERSE PROBLEM IN MARKOV MODELS.

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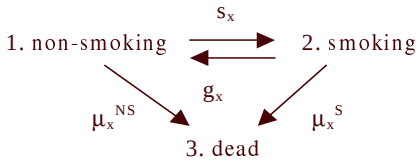
This paper considers decision of inverse problem of Markov model corresponding to a special insurance scheme.

Some applications consider the approach which use Markov theory to model situation as a multi-state process. For example, such cases can be problems of queuing theory, reliability theory etc. This approach receives wide using at actuarial practice where multi-state model applies to describe conditions of insuranced individual.
When modelling on the base of markov processes two mutually opposite problems arise. Direct problem is to calculate probabilities of corresponding states and other characteristics of process. It is assumed that parameters of model are available.
Inverse problem is to evaluate parameters of model by using experimental output data.
In markov model input parameters are forces of transition from state to state. When it concerns queuing problems or insurance models these values are unknown in advance. And statistical information about output data for some models can be found in special literature.
One of the useful methods to calculate probability of random event is markov scheme. But using markov models to insurance problems meet some difficulties. One of them is that system has too many possible states – conditions of individual health which depend on age and other characteristics. Errors of estimates can also depend on duration of insurance policy.
Approximation of markov system can be developed by consideration of some additional sub-states or subsystems. In case of life insurance it means that it will be necessary to separate individual age to periods on which forces of transition from state to state may be considered as constant.
When transition forces are available the case is leading to direct problem – decision of Kolmogorov-Chapmen equations. For models with constant forces it isn't very hard regardless the number of states. But if transition forces are unknown, inverse problem arises.
Thus in [1] multi-state model is used to describe processes of disability income insurance. Estimates of transition forces are obtained by means of maximum likelihood method. It is assumed availability of full information about history of each observed individual. That is all transition states and situated times of individual are known.
In life insurance problems experimental information is contained in so-called mortality tables which include data of mortality probability of individuals being in certain age and belonging to certain group.
The paper concerns decision of inverse problem on example of special case of insurance model.
Let's assume that individual can be in three states. Two of these are "alive" – "smoking" and "non-smoking", and one is "absorbing" – "dead". Scheme of transition is following:



The model has four unknown parameters (s_x, g_x, μ_x^{NS}, μ_x^{S}). It is available statistical information about probabilities of transitions from state 1 to state 3 and from state 2 to state 3 at age x. Values are taken from [2].
Considering various initial conditions and prescribed limitations by means of least squares method numerical estimations of transition forces are obtained.

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THREE-DIMENSIONAL MODEL OF NEAR OBJECTS USING VIDEOGRAMMETRY

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The methodology proposed in this investigation for the obtaining of the three-dimensional coordinates of the object, is not based on the well-known techniques of identification of homologous points, either in a manual way by means of stereoscopic vision, or automatic using on in technical of correlation of images. The principle of the developed method, consists on the study of the geometry that define all the edges of the object, in all the images that have him, to obtain its modeling one.

The problem consists in that a point of the edge with two coordinates, has to be defined a point of the model with three coordinates. The problem would be simple if we have the position of that same point in two frames (a point in two frames provides two coordinates ' x' and two coordinates ' y', that is to say, four data) however like we have proposed a point of the edge previously it only appears probably in only one frame, therefore the stereoscopic photogrammetry cannot be solved the problem. In principle the outlined problem is monoscopic.

The data obtained in the previous phases and that are needed to model the object are:

1) Parameters of external orientation of all the images, that is to say, the projection center (X0, Y0, Z0) and the rotation (w, f, k) of the camera in each taking point about the trajectory that will belong together with each one of the obtained images of the video sequence. Focal distance and radial distortion correction, besides other data that define the geometry of the video sequence.
2) The pixel coordinated (x, y) of the object edges in each one of the images.

With all these data we pretend to obtain in an automatic way, the three-dimensional model of the object and their precision. Also, the results are supplemented with the three-dimensional graphic exit by means of VRML, of the pattern obtained so much in format of wires, faces or textures

Initially we have for example 90.000 sectors of coordinates (Φ, H, ρ) where a initially taking a maximum value similar to the radius of the platform (0,5 m). According to the video taking we will have 1.500 images approximately recovering totally to the studied object (video of 60 seg. at 25 images per second). For each coordinated image Pi(x, y) belonging to a edge point in the image i [1, 1500] the following algorithm will be applied:

1) Calculation of the projected ray Ri (x, y) [1] that unites the projection center with the point of edge of pixel coordinates (x, and) on the image.
2) Calculation of the sectors that are intersected for the projected ray.
3) Calculation of the distance D to the center of the cylinder of each one of these sectors. If this distance is smaller to the coordinate ρ of this sector (initially equal to 0,5 m), then the value D is assigned to ρ.

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RESEARCH INTO INITIAL-BOUNDARY EFFECTS OF THE PHYSICAL PROCESSES

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Many physical processes are described with eliptic and parabolic equations. When solving eliptic equations in canonical domains with Dirichle boundary conditions by grids method, it is obvious, that boundary conditions are satisfied exactly. Therefore it should be expected that close to the domain boundary, accuracy of difference scheme should be higher than in the middle of the domain. This ideas arose during the work of V.L. Makarov together with R.D. Lazarov on their monograph [1]. The presence of such fact is quite natural and qualitatively was well known, because the error of the difference scheme for Dirichle's conditions equals zero, on the boundary of the canonical domain, but in quantitative formulation this fact for the first time was announced in [2].

In the series of our works with professor V. Makarov the accuracy estimates of difference scheme taking into account initial-boundary effect were studied. First, the three-point difference scheme of the nth order for the ordinary differential equations on uniform and non-uniform grid were studied. A priori estimates, which show, that accuracy of the difference scheme close to the domain boundary is higher, than in the middle were obtained. Numerical examples, which confirm theoretical conclusions were held.

As a development of the ideas mentioned above, a question arose: does the accuracy of differences schemes for parabolic equations increase close to $t = 0$, where initial conditions are given and close to boundary of canonical domain, where Dirichle conditions are given? Base for waiting for affirmative answer for the question put was that the error of difference schemes equals zero when $t = 0$ and on the domain's boundary. Such an affirmative answer for the linear case was found. The sufficient conditions of the incoming data smoothness (of the equation right side and initial conditions), which provide the validity of the a priori estimates mentioned above were determined. This conditions appear to be stronger than known conditions of smoothness [1], which provide coordinated estimates of the convergence speed of difference schemes for weak solutions, without taking into account initial-boundary effect. Further these results have been generalized on a case of bidimentional area.

Also estimates of the difference schemes accuracy for quasi-linear parabolic equations, which take into account initial-boundary effect were considered. For these equations 'weight' a priori estimates of the error, which quantitatively show on how much arises the order of accuracy of differences schemes on approach to the domain's boundary and in the initial moment of time, than in the middle of the area were found. Work on a numerical example is conducted.

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AN ENHANCED MATHEMATICAL PROGRAMMING MODEL FOR SCHEDULING THE GENERAL BATCH AND SEMICONTINOUS CHEMICAL PLANT

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In recent years, there has been an increased interest in batch/semi-continuous processes due to the increasing market share of high value added specialty products. Some of the products produced in batch plants include specialty chemicals, pharmaceuticals, biochemicals, and processed foods. Because typically these products are processed in small quantities, batch plants usually consist of general purpose equipment items. As a consequence, batch plants offer the prospect of producing several products in one plant by sharing the available production time between units. This sharing of resources necessitates the determination of the order or the schedule in which products are to be processed in each of the units of the plant so as to optimize some suitable economic or system performance criterion.

The solution of the scheduling problem is significantly affected by the structure of the processing network, the nature of intermediate storage between stages, the processing times for each product in each operation, the cost and time associated with product changeovers, and the performance criterion used to rank schedules. A procedure aiming to give a realistic solution to the scheduling problem must accommodate all of the above features.

This paper presents a novel mixed integer linear programming formulation that treats a wide variety of scheduling problems that involve both batch and semicontinuous processing. This formulation is based on a uniform discretization of time, has various advantages over models considered by previous researchers, and includes several extensions for handling deadline violations, semicontinuous processing units, and multipurpose storage vessels. Two types of due dates were considered: soft and hard. The present problem has a complex combinatorial nature with a moderate integrality gap. The solution increases rapidly with problem size. To be useful in industry, an efficient solution strategy is required. To this end, several computational as well as formulation aspects of this problem merit further study. The model presented in this paper provides a basis for such an algorithm that will be the focus of a companion paper.

Keywords: multiproduct and multipurpose plant, batch and semicontinuous unit, resource constrained scheduling, mixed integer programming.

PETRI NET BASED MODELLING AND PARALLEL SIMULATION OF CHEMICAL TECHNOLOGICAL SYSTEMS

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A wide class of chemical process operations, including batch processing, start up and shut down, are characterized by discrete process states and operations, therefore they can be modelled as discrete event systems. The description of operating procedures, i.e. the operations to be performed to make significant changes in operating conditions, is generally very complex; procedures always contain sequential and parallel actions, events and sub-processes. Due to their discrete character, chemical technological systems can be described with Petri nets [1].

Large systems modelled by Petri nets, however, can result in very large nets whose analysis and simulation are very time consuming. Often, the analysis is difficult to perform due to the combinatorial explosion of the state space. Parallel computing technologies can help in speeding up the execution of the simulation [2], but the design of a suitable parallel simulation program is a considerable task.

In this poster we report on our ongoing work that concentrates on modelling chemical technological systems with Petri nets and studying their potential and suitability for parallel simulation. We present a Petri net model of a given chemical technological system as an example for large complex systems. It contains several different kinds of technological units, such as reactors, distillation columns and their supplement units. The goal of the model development and the investigation is to identify suitable range of system parameter values that guarantees the continuous operation of the central system unit as well as the fulfilment of capacity demands. The Petri net model of this system contains about sixty places and transitions but if the sub-processes are modelled in detail, then the number of net elements can easily reach several hundreds. The example also shows that operating procedures of large processes exhibit a hierarchical nature: a typical plant-level or high level operating procedure includes operating procedures of unit level (i.e. lower level). The hierarchical Petri net model offers the possibility of examining and exploiting this hierarchical nature of the target system, and thus simplifying the analysis and verification of the operating procedures.

We have developed a sequential Petri net simulation program as well as parallelism analyser tool that helps in simplifying large Petri net simulations and creating efficient parallel implementations. The analyser uses run-time trace information obtained from a sequential run of the simulation, then -by analysing this trace- predicts the run-time behaviour and expected execution time of the parallel version of the simulation. If such an analysis demonstrates that the parallel execution can lead to a potentially more efficient and shorter execution of the simulation, the parallel version is worth developing. The mapping facility of the analyser can be used to identify those places and transitions that should be merged into spatial regions and then mapped to logical simulation processes. This granularity reduction is inevitable in order to achieve increased performance.

The poster describes the current results of our ongoing project. Our future work involves the modelling and analysis of more complex and larger chemical systems.

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OPTIMAL CONTROL MODEL OF ADVERTISING THE DURABLE GOODS, PROVIDED THE MARKET PARAMETERS ARE CHANGING OVER TIME

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The dynamics of advertising the durable goods is well described by the Bass equation [1] and by its subsequent versions [2,4]. The corresponding optimal control model is as follows: the state equation is the Bass equation, the state variable is the cumulative sales, the control variable u(t) is the advertising rate, U denotes the upper bound of this rate, the objective function to be maximized is the profits (the benefits minus the advertising expenditures), T is a fixed planning time of sales. It is easy to make sure that the maximum principle [3] results in the solution of this problem in closed form for the undiscounted case. It turns out that the optimal advertising policy is a kind of policy known as a bang-bang policy in the control theory literature. There exists a turnpike value θ of the time of sales T: if $T<\theta$ the optimal advertising rate is equal to its upper bound U all over the time of sales T (Fig.1), if $T>\theta$ this rate equals U only over the time interval $[0, \tau]$ and it is equal to zero over the time interval $(\tau, T]$ (Fig.2), the value τ being determined by the maximum principle as a function of T. It should be noted that τ is a decreasing function of T, θ and τ are obtained as the explicit functions of T.

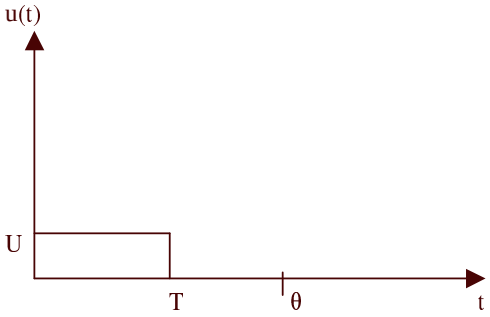

Fig.1. Optimal advertising rate ($T<\theta$).

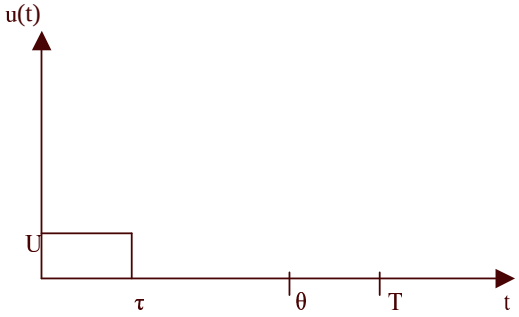

Fig. 2. Optimal advertising rate ($T>\theta$).

Unfortunately, this approach fails if the parameters of the Bass model are changing over time. The aim of this contribution is to construct a model of advertising under these circumstances. We apply the algorithm of forecasting model with a fixed programme of changing of the parameters [5] in the following way: the derivative of x with respect to time is considered as a new control variable, the objective function is the function of generalized work [5]. This approach is applied to the case of several different regions of advertising (the corresponding numerical examples are given for the cases of one and two regions).

Such an approach has the same important advantages the classical methods of the optimal control theory have (these methods are used in the framework of this approach in order to construct the base fixed programme). But this approach has an additional advantage: it permits to take into account the deviations of the system dynamics from the dynamics of the fixed programme in the real time.

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MODELLING OF INTENSITY DISTRIBUTION OF BISTATIC POLYDISPERSE LIGHT SCATTERING IN THE SEMICYLINDRICAL OPTICAL SENSOR OF POWDER MATERIALS' CHARACTERISTICS

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It is considered the problem of modelling and transformation of diffuse reflectance characteristics for polydisperse powder deposited or strewed onto the work surface of the optical sensor with the thick transparent substrate (fig.1), which was proposed in the author's earlier papers instead of sensors with preliminary dispersion of powder or passing the particles through the narrow channel. Since the diffusely reflected into substrate rays are registered by photocells on the flat bottom surface of this substrate (see fig.1), the diffuse reflectance characteristics must be finally transformed into the surface distribution function (SDF) of intensity of bistatic light scattering.

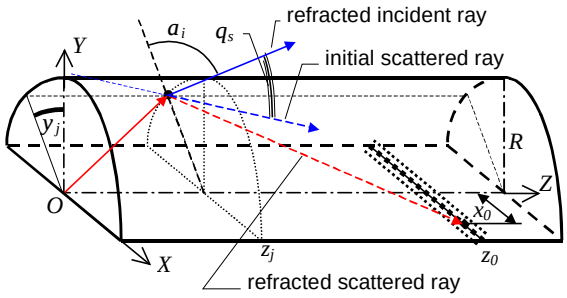

Fig.1. Rays configuration in the semicylindrical sensor.

Unfortunately, the rigorous methods of determination of bi-directional reflectance distribution function (BRDF) for polydisperse powders, based on the theory of elastic multiple light scattering, is too complicated. For this reason, the methods of Monte Carlo simulation are usually applied for solving of similar problems, as in [1,2]. But, the majority of known corresponding papers do not take into account the particle size distribution. Furthermore, the algorithms, which generates the random polar scattering angle by the probability density function, are often obliged to utilise too simplified Henyey-Greenstein phase function instead more accurate Mie phase function, as in [2]. Evidently, no papers perform final transformation of BRDF into SDF of intensity according to geometry of proposed sensor.

In this paper, the Monte Carlo simulation of SDF of bistatic scattering intensity is performed for polydisperse monolayer of powder particles on the work surface of semicylindrical sensor. The main steps of this simulation are:

1) Generation of random polydisperse monolayer of particles with corresponding binning and mapping of sensor's work surface.

2) Initialisation of photon packet with weight $w_j>>1$, with random enter point (z_j,y_j) into particle layer and with initial direction that is determined by angle a_{ij} (see fig.1) and corresponds to given enter point.

3) If coordinates (z_j,y_j) coincide with filled bins of work surface (the photon packet hits the particle), the direction of scattering is determined by the random polar and azimuthal scattering angles q_{sj}, j_{sj} **uniformly distributed** in $(0,p)$ and $(0,2p)$ respectively.

4) If given direction corresponds to the photocell with some coordinates (x_0,z_0) on the bottom surface of substrate or provides propagation within layer of particles, **the weight** w_j of photon packet **is changed proportionally to Mie phase function** for given particle size and scattering angle q_{sj}.

5) All photon packets reached the photocells are summed respectively for obtaining of intensity SDF. For the packets propagating within layer, the coordinates and bins for nearest particle (in the line of propagation) are determined for the 2nd scattering events and steps 3)–5) are repeated.

Data for construction of statistics are collected by repeated generation of the new monolayers of particles. The influence of disperse composition of powder is investigated.

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[1] Dr Ihor Ivasiv is an award holder of the NATO Science Fellowships Programme.

APPLICATION OF HIERARCHY OF TWO OBJECTIVE FUNCTIONS WITH SPIRAL FORECASTING MODEL TO THE PROBLEM OF AIRCRAFT LANDING

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When an aircraft is landing it is of great importance to provide the given values of its trajectory parameters and of its coordinates at the terminal time. This problem is rather complicated if it is solved by the methods of classical optimal control theory in the real time of landing due to the calculation difficulties. Particularly these difficulties arise when solving the two-point boundary value problem, connected with the necessity to search the field of shooting in parameters for which the iteration process converges. This field can be obtained by interpolation, for example. If the conditions of flight are changing during the aircraft landing all the calculations have to be carried out many times from the start, including the searching the initial approximation [1].

Application Krasovskii function of generalized work [1] and the corresponding algorithm with a forecasting model to this problem gives the compromised result from the point of view the landing accuracy determined by the given weighted coefficients of the terminal part of objective function. The investigation shows that for providing the safe landing one should apply an algorithm of step by step optimization according to the hierarchy of the objective functions over the unfixed time interval [2]. In this case the terminal requirements for the angle coordinates of the aircraft are contained in the objective function of upper level. The linear deviations from the given terminal coordinates of the aircraft are contained in the objective function of second level. In this algorithm the aircraft is considered as a solid body in the body axis system. The forecasting terminal values of the aircraft state vector are obtained in closed form, the overcharging and the angle velocity being supposed to be constant. This model is called the model of spiral forecasting. It permits to provide the optimal control on board during landing. The adjoin variables necessary for finding the optimal control are calculated numerically, provided the integrand Q(x, t) of the minimized objective function differs from zero (x is n-dimensional state vector, t-time). It should be noted that this integrand determines the quality of the change over processes. Apart from that the alternative version of considered algorithm is constructed. In this version the case with Q unequal to zero is reduced to the case with Q equal to zero by means of introducing an additional control variable the derivative of which with respect to time equals the integrand Q. This approach makes it possible to obtain the control in closed form. The calculations carried out according to these versions of the constructed algorithm show the effectiveness of this algorithm (Fig.1.).

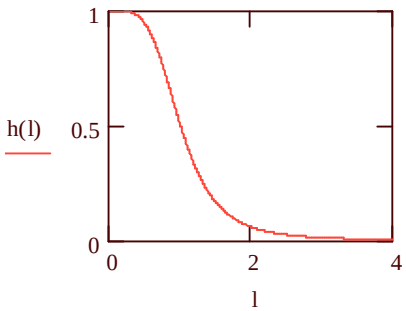

Fig.1. The trajectory of aircraft landing (h-altitude and l-distance of landing in km).

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STATE ESTIMATION FOR MONITORING AND CONTROLING

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In biochemical pollution modelling with using only biochemical oxygen demand (BOD) and dissolved oxygen (DO) river can be treated as cascade of objects with distributed parameters, which is described by first order hyperbolic equations of transportation type. Object described by first order partial differential equations can be substituted by set of ordinary differential equations with discrete measurements in the time domain. It is possible with different object interpretation then up to now. The main idea of such approach is consideration of the process along lines connected to moving speed of coordinates of state vector in object. It responds especially to object such river. That interpretation brings description of object to consideration of large number of characteristics, which cover whole space. State of polluted river described by differential equation of transportation type, while considering function along characteristics, can be described by infinity number of ordinary differential equation. In such case measurements become discrete in time [1]. It is necessary to know characteristics of signals (expressed in formulas as covariance**)**, which influence on object. In practise it is difficult to obtain. For practical realization the idea of joining filtration and prediction artificial neural network can be used. We can expect that well worked out artificial neural network allows avoid difficulties of classical filtration approach. The design of two separate artificial neural networks realizing both phases of estimation gave satisfactory results. Using artificial neural network in filtration and prediction phase improved accuracy of estimation process. Net gives more precise estimates of river state than classical filter. Most rivers have systems of sewage treatment plants along them. In spite of that untreated sewage still flow into local surface water, what can causes big problems in some places. Main reasons are storms and damages of treatment plans. To avoid ecological disaster we need monitoring and controlling system. It's mean that we should interfere directly into river. The control has no effect on the variable, which represents in stream BOD level. Realisation of classical control system based only on one variable (DO) cannot preserve ecological crash. For example when into river flown pollution with high BOD level. Then DO level starts decrease. When DO level reaches warning level system will start supply oxygen directly into water. But it's to late to improve DO level in that part of water, so fishes and other aquatic life can died, if it fallen bellow minimum needed for survival. That's why information about BOD level is necessary. Measurements of BOD are not useful because they are long time consuming (5 or 25 days). That is why we need estimation process. System with estimation process has complete variables and can react on sudden drop of intensive pollution. Proposed monitoring and controlling system is shown on Fig.1.

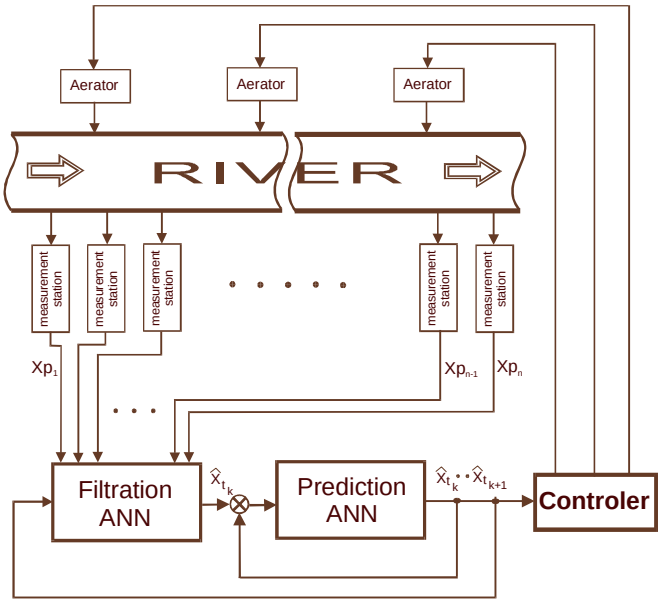

Fig.1. Scheme of monitoring and controlling system**.**

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MEDICAL EDUCATION VIA WWW BASED ON CONTINUOUS PHYSIOLOGICAL MODELS

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At the medical faculty of Graz University a new Curriculum has been developed for the studies of human medicine. This totally new approach is based on a Module-/Track-model and follows the basic principles of interdisciplinary, topic centered and patient oriented instruction. The Virtual Medical Campus general objective is the realization of an Information-system to make the curriculum digitally accessible. The learning objects used within this campus are developed on accepted standards for "trans-national education" as a basis for international networking in the form of Reusable Learning Objects. Reusable Learning objects (RLO) are elements of a new type of computer-based instruction grounded in the object-oriented paradigm of computer science. Object-orientation highly values the creation of components (called "objects") that can be reused (Dahl & Nygaard, 1966). The fundamental idea behind learning objects is that instructional designers can build small (relative to the size of an entire course) instructional components that can be reused a number of times in different contexts. Additionally, learning objects are generally understood to be digital entities deliverable over the Internet, meaning that any number of people can access and use them simultaneously (as opposed to traditional instructional media, such as an overhead or video tape, which can only exist in one place at a time). Moreover, those who incorporate learning objects can collaborate on and benefit immediately from new versions. This is a significant difference between learning objects and other types of instructional media that have existed previously.

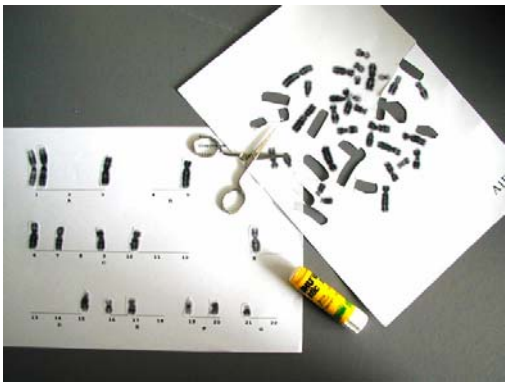

Fig. 1: Paperwork

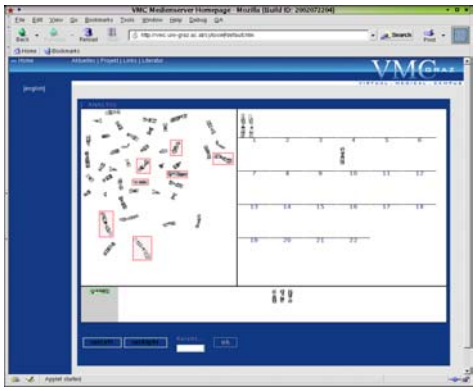

Fig. 2: Online Simulation

As an example we have chosen the field of cytogenetics. Cytogenetic analysis is an essential part of diagnostics in dysmorphology, syndromology, prenatal and developmental diagnosis, reproductive medicine, neuro-pediatrics, hematology, and oncology. Currently cytogenetic analysis is represented in the curriculum in a practical exercises unit. We use photographic material of microscope g-banded metaphases. Every student gets a photograph of a normal as well as a pathological metaphase and has to cut out the chromosomes manually to re-arrange them in the form of a karyotype. In routine analysis this manual procedure has been replaced by computer based analysis tools. These analysis tools have been designed to fulfill the complex requirements of routine analysis and are therefore not practical for educational use. So the idea emerged, to develop an Internet enabled simulation tool in the form of a LO, which is reduced to the parts of didactic functionality. In the new curriculum we subsequently will keep the manual procedure for the normal karyotype to get in touch with the topic, but for the pathological cases we utilize a web based simulator of a cytogenetic analyze tool.

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ARTIFICIAL NEURAL NETWORK IN DIAGNOSTIC PROBLEMS OF RECTIFIER SYSTEM

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Rectifier systems are used in different fields of present life. Usually using time of electronic devices depends on proper work of supplying system, in which the main component is rectifier system. Moreover incorrect functioning of rectifier system can produce damage whole electronics sets. In the paper diagnostic of rectifier system with Artificial Neural Network (ANN) applying is proposed. Different architectures and work ideas of ANN were tested it i.e., linear ANN with classical back propagation learning method, Learning Vector Quantization Networks (LVQ) and Radial Basis Function (RBF). Proposed diagnostic system is easy to perform, no invading and allows receiving instant results. The working idea of example diagnostic system is shown on Fig. 1.

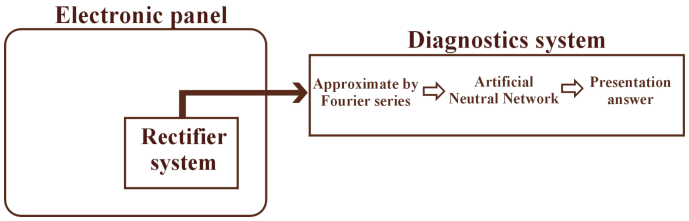

Fig. 1. Scheme of diagnostic system

Rectifier systems can have different configuration of diodes and thirystors. The current signal from rectifying elements is given on input of passive filters with RC, RL, and RLC character. Next the current flow to receiver. The current or voltage signal on receiver is the input signal for the diagnostic system, which main element is neural network. Examinations were carried out in Matlab environment. In that environment mathematical equations of rectifier system were modeled and the architecture of neural network were projected.
Simulation concerned different configuration of the rectifier system and values of parameters. Time signals of current and voltage on particular elements are final results. Obtained time signals in rectifier system were compatible with expectation. The artificial neural network, which is main element of diagnostic system, recognized different state of examined rectifier systems. The following cases of ANN were considered:

- with classical learning method (back propagation), where measurements from output of rectifier system are submitted for data preprocessing. Preprocessing was realized by Fourier series approximation on signal from rectifier system. In experiments different degree of approximation was applied. Values of amplitudes, phases of harmonics and constant were input signal for neural network. Number of neurons in input layer was determinate by degree of approximation. Feed forward ANN with different number of neurons in hidden layer was proposed and examined. More complex network required longer learning process. In investigations correct results were obtain. ANN generates answers about actual state of rectifier system with small error. Different result for differ architectures of ANN where obtained [1], [2].
- with direct measurement of diagnosing rectifier system without necessity of data preprocessing. Learning Vector Quantization Networks were using for that purpose. The LVQ consist of two layers, rivaling (Kohonen) and classifying one. Size of input vector determines number of neurons in input layer. User defines number of neurons in Kohonen layer. Second layer (output) has as many neurons as many signals need to be recognized. ANN classified recognized signals to particular class. Thus structure of ANN depends as well on number of classes. Net correctly classified configurations of rectifier system to proper signal classes. Analyzed signals were sampling with different frequency [3].
- without data preprocessing, Radial Basis Function, where neurons in hidden layer have radial transfer function. In case of radial function applying bigger diversity of shape selection take place. The most popular equivalent of signoidal function is here Gauss base function. The ANN with such architecture gives proper results of rectifier system identification.

The LVQ neural network gives better results than another examined ANN and allows obtain better distribution parameters of rectifier system diagnostic. The structure depends on input and output signals and is automatically chosen. Thus we can draw conclusion that kind of nets is perfect to solution problems of rectifier systems diagnostic Seems that presented conception can be successfully applying in practice.

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GENETIC ALGORITHMS FOR OPTIMISATION IN MODELS OF DISCRETE PROCESSES – AN EXCEL-BASED APPROACH

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David E. Goldberg – one of the fathers of Genetic Algorithms – named 1989 in his book "Genetic Algorithms in Search, Optimization, and Machine Learning" five reasons why handlers should deal with Genetic Algorithms:

- Genetic Algorithms are new and interesting. They are attracting attention in the academic world.
- Genetic Algorithms use search algorithms like nature does.
- Genetic Algorithms can be used for a number of problems.
- Genetic Algorithms are robust, efficient and they yield always the same solution quality.
- To use one method for a number of problems is more favourable than to use one single method for each class of problems.

Today Genetic Algorithms lost its importance. Nevertheless their characteristics convinced us when we searched for an algorithm for optimization for our problem.
The goal of the work was to generate an optimization module for the discrete simulator ED (Enterprise Dynamics), based on cost functions calculated from dynamic simulations. The implementation of the algorithm should be very general because the algorithm should be used for several problems. The use of the algorithm should also be very simple.

In Genetic Algorithms parameter samples are transformed into binary strings (genotypes) and for each of these genotypes a fitness value is computed with simulation. The fittest genotypes will be crossed (crossover) and will be fed back into the system again. Generally these children yield to better solutions. The solutions may be better solutions but they need not to be the best global solution. Maybe the initial population represents only a part of the parameter space. Therefore a mutation rate is introduced. With this rate new genotypes are created, so that it is possible to search an even larger parameter space.

Because it is very elaborately to generate new genotypes, it seams useful to perform this task in an external application, while the simulation itself runs in ED. Because of the comfortable DDE interface it was decided to use Excel to implement the Genetic Algorithm. A further advantage is, that this Excel-module can be used with every version of ED supporting DDE, and also for other simulators.

To enable a transparent data transfer, a high level module was implemented in ED, based on an extension of ED's experiment-module. On the one hand is should be simple to use and on the other it should transfer the fitness values from ED to Excel and the parameter values from Excel to ED. The user has only to fill out the basics for the Genetic Algorithm and to run the simulation. The Genetic Algorithm will do the rest further on.

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HIERARCHICAL TEMPLATES FOR SIMULATED INTELLIGENCE

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Abstract: We are intelligent, so we are conscient. We are in evolution, so we construct. We are not alone, so we have to contribute. Intelligence = (adaptability, conscience, intention) is complementary to faith = (intuition, inspiration, imagination). Conscience simulation demands transcending the present limits of computability, by an intensive effort on extensive research to integrate essential physical and mathematical knowledge guided by philosophical goals. A way to begin is hierarchical reconfigurable hard-soft cosimulation.

1. Introduction

Algorithms, designs, artificial systems can be computer simulated so they represent computability, bottom-up (construction, design, plan) or top-down (understanding, verification, learning). The algorithmic approach is equivalent to the formal one. Knowledge and construction hierarchies can cooperate to integrate design and verification into simulation: structural symbolic object-oriented concepts handle data and operations formally.

2. Hierarchical Approach

Coexistent interdependent hierarchies structure the universe of models for complex systems, e.g., hard-soft ones. Different hierarchy types are defined by abstraction levels, block structures, class network, symbolization and knowledge abstractions. Hierarchies of different types correspond to the kind of abstraction they reflect ( ):

Class hierarchy (concepts) virtual framework to represent any kind of hierarchy.
Symbolization hierarchy (mathematics) stepwise formalism for all kind of types, including hierarchy types.
Structure hierarchy (managing) stepwise managing of all (other hierarchy) types on different levels.
Construction hierarchy (simulation) simulation (=design/ verification) framework of autonomous levels.
Knowledge hierarchy (theories) reflexive abstraction: each level knows its inferior levels, including itself.

The hierarchy types can be formalized in the theory of categories [1]. Constructive type theory permits formal simulation by generating an object satisfying the specification. A generic type is the ability to parameterize with types a hardware/ software element. Recurrence is confined to discrete worlds, while abstraction is not. This suggests searching for understanding following mathematical structures that order algebra into topology [2]. *Reality is beyond nature* (IN IR). We follow the paradigm of intelligent simulation by functionally modeling the self-aware adaptable behavior for intelligence simulation. The integration between discrete and analog is needed [3], for a softer adaptability and for conscience simulation as analog reaction. Recurrence of structures and operations enables approximate self-knowledge, with improved precision on the higher knowledge levels. A hierarchical formal system is defined by hierarchical universe, functional objects, initial functions and transformation rules. Integrating algebra, topology and order, functional analysis contains appropriate structures for self-referent models: contractions and fixed points in metric spaces, reflexive normed vector spaces, inductive limits of locally convex spaces, self-adjoint operators of Hilbert spaces, inversable operators in Banach algebra. *Simulability is computability using the power of continuum.*

3. Conclusions and plans

We enrich the template concept to structures and create a theoretical kernel, for self-organizing systems, based on a hierarchical formalism. This permits theoretical development as well as efficient application to different cosimulation types of reconfigurable systems. Further than modeling conscience to simulate intelligence there will be search to comprehend inspiration maybe using Lebesgue measure on differentiable manifolds and/or non-separable Hilbert spaces. Even mathematics will have to develop more philosophy-oriented to approach intuition.

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CONTROL SYSTEM DYNAMIC MODEL CONSTRUCTION WITH FUZZY PHASE LIMITATIONS FORMED BY USING AN ENTRY MEASURE OF AFFINITY

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Effective control laws forming for various dynamic objects is one of the modern engineering major problems. Numerous works are devoted to its solution. Thus main difficulties for control law forming can be met, when for dynamic object moving control it is necessary to provide various limitations: on a motion path, on values and structure of control. It is also necessary to take into account object parameters spread, the incomplete information on acting disturbances. It is also difficult enough to provide the requirement of real time control synthesis. To overcome the specified difficulties in works [1], [2] the method of phase limitations variation is offered. In the given paper the method generalization and the further development is considered, which allows to expand set of possible solutions and to take into account the various limitations. According to the approach for dynamic object, described by the equation: $\dot{x} = f(x,u,v,t)$ (x,u,v are the vectors of a condition, control, disturbances), - the so-called measure (function) of affinity $\rho(x,Q)$ is entered. The given function determines a affinity degree of point x location towards some given set Q which characterizes phase limitations on dynamic object trajectories. And the affinity x to Q can be understood, as directly according to the using metrics in the state space R^n (i.e. as distance from point to the set), and in more general case, as some scalar value set by entered function (or by functional), determined on elements R^n and Q and establishing between them and the specified value the correspondence.

The synthesis task is providing of the given phase limitations at presence of various requirements to dynamic object. Due to the fact that the "rigid" phase limitations lead to the unsolvability of a synthesis task it is offered to set limitations on a condition vector in the fuzzy way:

$$\rho(x(t),Q) \le \varepsilon \tag{1}$$

where non-negative scalar value ε characterizes a degree of fuzziness ("thickness" of phase limitations border).It is possible to show, that for fuzzy phase limitations providing of a considered type the following inequality should be fulfilled:

$$\left.\begin{array}{l}(\nabla_x\rho + (\nabla_x\xi)^T \cdot \nabla_s\rho,\, f(\cdot)) + (\nabla_s\rho, \dfrac{\partial\xi}{\partial t}) \le 0 \\ \forall s \in \Gamma Q(t), \quad x = x(s,\varepsilon)\end{array}\right\} \tag{2}$$

Here $\Gamma Q(t)$ is border of set $Q(t)$; (α,β) - scalar product of vectors α and β, $\nabla_x\rho, \nabla_s\rho$ - gradients of function ρ on a variables x and s; vector $s \in \Gamma Q(t)$ is uniquely determined for every $x \notin Q(t)$ according to that sense which function $\rho(\cdot)$ has, i.e. $\rho(x,Q) = \rho(x,s)$

And $s = \xi(x,t)$ - analytically determined function; under $x(s,\varepsilon)$ the uniquely determined element $x \notin Q$ is meant in sense of the entered function $\rho(\cdot)$ and this element corresponds to the given s and ε.

The obtained inequality (2) effectively allows to take into account various limitations for the given task and supports the solution in a real time mode.

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ANALYSIS OF MULTILINEAR SYSTEMS USING GRÖBNER-BASES OVER THE FINITE FIELD $\mathbb{F}_2$[1]

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Striving for an exact solution of systems of polynomial equations Gröbner-bases are known to be an appropriate representation for these systems on the field of real numbers [1]. By the use of Buchberger's algorithm those systems of polynomial equations are transformed into an other, in a sense simpler, set of polynomials without changing the variety, that is the solution set of the system. This set of polynomials forms the so-called Gröbner-base. Gröbner-bases show the following very advantageous properties:

1. Referring to a certain term ordering the underlying polynomials of the Gröbner-base are in triangular form; very similar to linear systems of equations after execution of the Gaussian Algorithm.
2. Gröbner-bases immediately indicate whether the system of polynomial equations is solvable or not.
3. The calculation of Gröbner-bases takes finitely many steps of algebraic computation.

The first property, the elimination property, guarantees (under minor assumptions) that an n-dimensional system of polynomial equations over the field of real numbers with n unknowns can be solved by first calculating the roots of an univariate polynomial (the n-th equation), which then are consequently available for a simple backward substitution process. Presupposing that this n-th polynomial equation is univariate and of at most fourth degree the solution set of the system can be evaluated in an exact, analytical manor, without employing any numerics. In nonlinear control system analysis and design Gröbner-bases have been used for finding equilibria and periodic solutions, for estimating the domain of attraction and testing for controllability and observability [4]. In the case of finite fields many of the presented ideas hold almost as they stand for real numbers. Some obstacles even disappear within the finite field case, for example rounding errors. By modeling finite state automata over the finite field $\mathbb{F}_2$, in general multilinear[2], hence polynomial systems are obtained. Thus Gröbner-bases prove to be properly tailored for analyzing automata in the finite field framework, as shown by [2,3]. In this contribution, first of all Gröbner-bases over finite fields and their special properties are developed (e.g. zero polynomials, irreducibility, quotient rings). By adaption of Buchberger's algorithm to finite fields Gröbner-bases for polynomial systems over finite fields are derived. Reduced Gröbner-bases are motivated in order to obtain a unique, canonical representation of the polynomial system, which allows of showing equivalence of systems. Using Gröbner-bases the analysis problem for cyclic states is solved for general, multilinear autonomous systems. Finally some remarks are cited as first steps towards a feedback design for these systems.

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OPTIMAL CONTROL OF ENTERPRISE WITH SELF-ORGANIZING MODELS

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Globalisation of financial and commodity markets in the world creates a dynamic and highly volatile economical environment. The problem of enterprise's sustainable development in such conditions raises the question of development of the optimal control. But the enterprise as a socio-economic system creates substantial difficulties owing to formalisation and transaction from the informal requirements to the optimality criterion defined in mathematical terms.

Construction of a reliable managerial strategy for the enterprise under the condition of competitive economy, insufficient and rapidly becoming out of date information demands the development of a new method, which possess to work in a dynamic, indefinite and fuzzy environment. For solving this problem it is recommended to make use of the algorithms based on the theory of self-organising optimal extrapolating controllers (SOEC) [1 – 3]. Developed at first for solving the problem of control of the flying object, these algorithms were approved lately to be effective for some socio-economic systems. The major advantage of the algorithms suggested is that they can be used for control of multi-dimensional objects in absence of the appropriate mathematical model of the controlled system.

The aim of the research was to adapt the algorithms with self-organisation to the development of optimal control of turbine manufacturing company (JSC "Leningradskij Metallicheskij Zavod" – the biggest Russian manufacturer of stem turbines for SPP). The problem of enterprise's control can be solved using the SOEC. Gross revenue Y was taken as the system's output, assets $\{A_i\}$ and the number of manufacturing personnel N were taken as the system's inputs. Budgeting constraints restrict the controlled process. These constraints consist of the personnel expenditures, the upper limit of investments into fixed assets renovation and the overall expenditures. Let us take a functional that links Y with A_i and N as an optimality criterion. The terminal part of functional includes deviation of the production output from its planned value, whilst the integral part of a functional includes a penalty function for exceeding the budgeting constrains and allowed costs of control. The data on measurements of outputs and the information of inputs for previous years are available. In our computations we used the hypothetical data for the production output (per years). The results of computation for the initial conditions at the input $A_1 = 2511145$, $A_2 = 953867$, $N = 7650$, and the information on the output for the last 5 years 723310, 800388, 1675357, 2323686, 2458204 show the effective usage of incoming information and possess us to maintain enterprise production output in accordance with the chosen criterion.

The computation conducted demonstrates the excision dynamics of rise in production compared with that when the algorithms with self-organisation were not used.

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DYNAMIC AUTOMATISED GENERATION OF DISCRETE PROCESS FLOW MODELS IN OBJECT-ORIENTED SIMULATORS

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In the course of developing an Simulation of the production plant of Radex Heraclit Industries (RHI) two main problems quickly surfaced: There was an extremely high amount of input data needed and furthermore the simulation should offer the possibility to simulate different scenarios, i.e. removing or adding machines to the system.
The production plant considered in this project consists of a large amount of machines and a complex course of production depending on part number, the availability of preprocessed parts needed, the availability of machines needed, temperature of manufacturing.
Additionally, following points needed to be taken in consideration:

- A high number of different products each of them taking a different course of manufacture
- Two different kinds of machines need to be distinguished: working places and furnaces
- Storages between each step of manufacture
- Furnaces can switch between different temperatures.

The input consists of two kinds of products: those who require preprocessed parts and those who do not. Products are loaded unto pallets with a maximum weight of 250 kg.

The Simulation

The simulation was done in Enterprise Dynamics 4.0 due to its open structure and 4d script that offers a very high flexibility as well as an ODBC interface.
According to a production plan the number of raw products to be produced each day is created. This may be up to several thousand on one day. Due to this high number of products in the system only pallets of products are considered.

Input From Database

The high amount of data needed for this simulation was stored in an Access database.
System related Data: Number of working places and furnace, A list of all temperatures at that furnaces can go, Changes in the number of tours for single machines, machine up and down times, way of manufacture for all products depending on part number
Machine Related Data: machine name, transport time from and to storage, machine category, capacity, capacity of furnace cars, spoilage, clock cycle of furnace cars, waiting time, number of tours per day, cycle time depending on part number and machine category

Generation of the Simulation

As soon as all data is received the final structure of the simulation forms itself automatically. 150 working places and 50 furnaces basically already exist. According to the imported data the required number of furnaces and working places are parameterised and connected to the system. For each activated machine a monitor is created to display their status during simulation.
In front of each furnace a storage is created. Each pallet is assigned a label on creation, containing the temperature the products it carries will need. According to this they are stored.

Results

The main goal of this project was to create a simulation that offers the possibility to change the structure of the model by adding machines and furnaces and change system parameters. The large amount of data needed implied the use of a database connected to the simulation. This resulted in a simulation that not only imported the needed data for simulating but also data concerning the whole model structure. Only a basic structure is implemented and according to the data imported from the database the full simulation model is created on resetting. This offers a high flexibility: machines can be added and removed, parameters changed as well as the whole course of manufacture only by editing the corresponding data in the database. The data collected during simulation allows a precise analysis and comparison of single simulation runs.

Parallel Computations Based on the Taylor Series Method

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A new version of the simulation language TKSL/C for extremely exact, stable, robust and fast numerical solutions of large systems of ordinary differential equations has been created. The algorithm of the solution is based on the Taylor series method. Positive properties of the method and some test examples of the Taylor series method are presented together with possible applications.
In a natural way, the Taylor series method involves solutions of problems that can be reduced (transformed) into solving a system of differential equations. That is why large systems of linear algebraic equations, partial differential equations and roots of algebraic equations are delt with.

It is characteristic of the Modern Taylor Series Method that the computation accuracy for a given step length is increased with the number of Taylor series terms used. However this increase in accuracy is not unlimited. For a given integration step length, there is always a saturated computation error that depends on the arithmetic unit word length. In some cases this saturated computation error can be reduced by decreasing the integration step or increasing the arithmetic unit word length. The effect of increasing the arithmetic unit word is more significant than that of reducing the integration step length.
It is the aim of the paper to design a special multiprocessor parallel system working with the arbitrary arithmetic unit word length.

The Modern Taylor Seriers Method also has some properties very favourable for parallel processing. Many calculation operations are independent making it possible to perform the calculations independently using separate processors of parallel computing systems. This parallel approach will be tested in a special gate arrays.

Since the calculations of the transformed system (after the automatic transformation of the initial problem) use only the basic mathematical operations (+,-,*,/), simple specialised elementary processors can be designed for their implementation thus creating an efficient parallel computing system with a relatively simple architecture.

[1]Brno University of Technology, Brno, Czech Republic, `http://www.fit.vutbr.cz`
[2]Ondemand GmBH, Wien, Austria, `http://www.ondemand.co.at`

ON THE ONE-DIMENSIONAL MODELLING OF HUMAN ARTERIAL BLOOD FLOW

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The growing interest in the mathematical modelling of the cardiovascular system leaded to numerous works which have appeard in the past, for example [1,2,3,4] and references therein. The application of simplified models have been shown to provide useful information for engineers and practitioners at reasonable computational cost. This paper deals with the analysis of the modelling of a simplified one-dimensional model of the cardiovasular system. The modelisation procedure is carried out in two different ways: first asymptotic reduction of the Navier-Stokes equations is used and second the derivation via the integral formulation of mass and momentum balance. Because some inconsistencies occured in the past we point out the details of the derivation of the balance law. Equipped with boundary conditions we show the stability of the system of partial differential equations even in the case of space varying parameters such as tapering of vessels and varying elasticities. Furthermore we give a mathematical analysis of the first occurence of shock waves in the cardiovascular system. Additionally we show how the balance law can be treated in a very efficient way by the use of finite volume and adopted central differences schemes.
We analyse disturbances whose wavelength are much greater than the vessel diameter, so that the time-dependent internal pressure can be taken to be a function only of longitudinal coordinate x and time t. The disturbed corss-sectional area is denoted by A(x,t) and the volume flow Q(x,t). Thus the model is one-dimensional. Starting from an axisymmetric tube and the Navier-Stokes equations in cylindrical coordinates dimensional analysis and scaling give the following equations

$$\frac{\partial A(x,t)}{\partial t} + \frac{\partial Q(x,t)}{\partial x} = 0$$
$$\frac{\partial Q(x,t)}{\partial t} + \frac{\partial}{\partial x}\left(\alpha \frac{Q^2(x,t)}{A(x,t)}\right) + \frac{A(x,t)}{\rho}\frac{\partial p(x,t)}{\partial x} = R(Q,A),$$

where ρ is the density, α a coefficient concerning he non-flat velocity profile, p(x,t) the internal pressure and R(Q,A) a term regarding the viscosity of blood. It will be shown that the same equations can be derived taking the integral formulation of mass and balance equations under the assumption of small vessel area changes compared to the inital tube diameter. An additional state equation for the elastic properties of the arterial wall gives the missing third equation. Several elasticity models for the vessel wall are discussed. All together we obtain a conservation law which can be expressed in conservative form. Because we take tapering and locally stiffed arteries into account the conservation law has a sourceterm and a flux function which explicitely depends on the space variable x. Furthermore three different types of boundary conditions occur in the arterial tree. The blood flow at the left heart valve, bifurcations of arteries and the distal (artificial) ends of the arterial tree are modelled by the help of Windkessel terminals.
By the use of the Energy Method we obtain stability results of the governing boundary value problem. First the stability regarding a single tube is discussed. Based on this analysis we obtain the stability of the full nonlinear boundary value problem. Thus the stability arguments can be extended to the whole arterial tree. A detailed analysis of the structure of the Riemann Invariants of the give balance law we obtain estimates about the first occurence of shock waves.
The contribution presents recent developed finite volume schemes for balance laws, giving same results but being more efficient than other schemes used.

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VIDEOGRAMMETRY SYSTEM ORIENTATION

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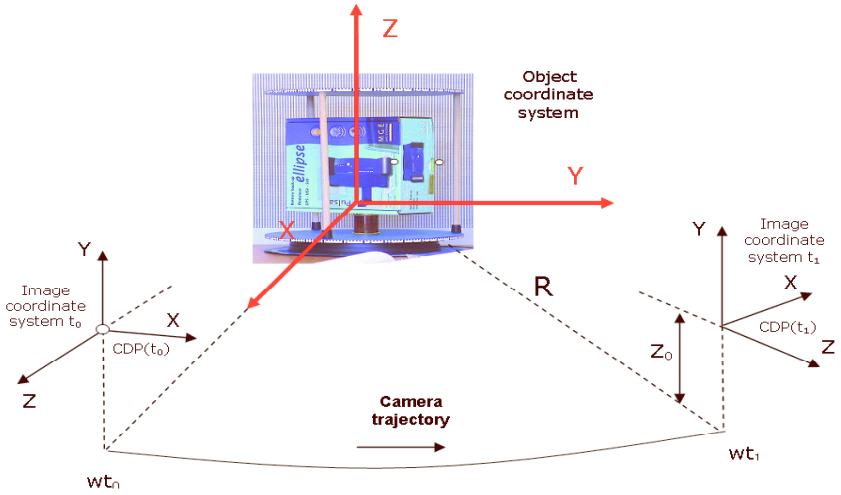
For to model an small object size by means of mosnoscopic and stereoscopic photogrammetric processes , the part of image of the frame is only used in the one that is contained the object, so that the image part that doesn't contain to the object it is not profitable.

In this abstract an alternative is presented to the terrestrial photogrammetry or the laser systems, to obtain the complete modeling of near objects in an automated way, only using the part of the corresponding image on the object edge.

Because the border of the object contains very little information, it is necessary to have many photogrammetric takings that provide many sections (in fact they are not properly sections, they are projections of the object contour). As the simplest photographic instrument to obtain many photogrammetric takings is the videotape camera, it will be the instrument used in this research, although the conclusions obtained are not limited to this type of images. Perfectly we could be used a digital photographic camera and a good image sequence that it recovers the object completely.

The work that we propose consists on eliminating of the constructive pattern the part that he has more than enough for comparison with the image of the border. The process can define it as a refined sustractive of the constructive pattern. This way, each point of the modeling end of the object was defined by a series of right encircling that they will locate it in the space, and they will characterize it in precision, without the identification in any case of homologous points.The reach of this investigation will be to study the possibilities of the method and its limitations. In the study they were proven the obtained precisions. In the case that we were limitations to this method, we will be studied different alternative possible proposing solutions for these cases.

The phases of the process are: 1) System object variables.Variables that define the geometry of the revolvable support. 2) Optimal obtaining of the video taking in function of the conditions of brightness, focus, color, etc. 3) Definition of the system geometry, parameters phptogrammetric of the camera, [1]. 4) Variables and calculation the trajectory of the taking. 5) Automatic obtaining the borders of the object. 6) Refined of the constructive pattern. 7) Evaluation of the precision of the refined model. 8) The study of the method limitations and their automatic detection. 9) Improves of the model with other techniques.



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