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GEOMETRIC REDUCTION OF DISTRIBUTED PARAMETER SYSTEMS USING PSEUDO-SPECTRAL METHODS

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Abstract.

A reduction method which preserves geometric structure and energetic properties of non linear distributed parameter systems is presented. It is stated as a general pseudo-spectral method using approximation spaces generated by polynomials bases. It applies to Hamiltonian formulations of distributed parameter systems which may be derived for hyperbolic systems (wave equation, beam model, shallow water model) as well as for parabolic ones (heat or diffusion equations, reaction-diffusion models). It is defined in order to preserve the geometric symplectic interconnection structure (Stokes-Dirac structure) of the infinite dimensional model by performing exact differentiation and by a suitable choice of port-variables. This leads to a reduced port-controlled Hamiltonian finite-dimensional system of ordinary differential equations. Moreover the stored and dissipated power in the reduced model are approximations of the distributed ones. The method thus allows the direct use of thermodynamics phenomenological constitutive equations for the design of passivity-based or energy shaping control techniques.

1 Introduction

Port-based modelling techniques and languages have been extensively used these last decades to model, simulate and control a wide variety of lumped parameters physical systems [6]. More recently extensions have been proposed for distributed parameters systems. They were first "series"-like expansions models derived from various kind of finite differences or finite elements methods. These already appear in many textbooks such as [6]. But "real" infinite dimensional port-based models for systems with boundary energy flow have also been proposed. They are based on the definition of the states as densities of some thermodynamical extensive variables. These state variables are related together through phenomenological constitutive equations and geometric interconnection structures [7]. Very recently this modelling approach has been applied successfully to many hyperbolic systems as varied as transmission lines models [8], beam equations [9] or shallow water equations [10]. The approach has also been applied to parabolic model such as in [11] for heat and mass transport models in an adsorption column, [12] for fuel cell models or [13] for multi-scale diffusion models. We may conclude from all these works that this modelling approach is pertaining to handle distributed parameter systems where classical thermodynamics applies. In this sense, the port-controlled Hamiltonian approach extents classical results from system theory to infinite dimensional systems.

Either for simulation or control purposes, distributed parameters systems (systems of partial differential state equations) are usually reduced or simplified in some way and most often turned into finite dimensional approximations. In this paper we are interested in the reduction to continuous time finite dimensional state space systems. The most popular methods to perform this partial (spatial) discretization are finite differences methods, finite elements methods and pseudo-spectral methods (see [14] for a large introduction to all of these methods and more specifically [15, 16] for pseudospectral methods). Recently Proper Orthogonal Decomposition (POD) methods have also been developed and applied to model reduction in an "identification for control" context (see [17] for linear system identification and [18] for control of non linear PDEs). However, these POD methods are rather designed for signal (image) analysis and their dynamical properties are far from well-known.

In this paper we are interested in reduction schemes which both preserve the geometric interconnection structure of our infinite dimensional model and approximate the energetic behavior of the actual system. This means that in the lossless case some approximated extensive variables will be conserved (as a first integral) and that the dissipated power will be approximated conveniently. Finite difference schemes are often used by specialist of application domains but in very specific formulations and they seldom lead to general formulation with such desired geometric and energetic properties. Finite element methods have already been adapted to lead to such formulation. First applied to electromagnetism problems [19], mixed finite elements formulations have been successfully applied to various Hamiltonian formulation of distributed parameter systems such as transmission line [8], diffusion problems [20] and shallow water fluid dynamics [21].

However in many applications, pseudospectral methods are preferred because they lead to low order approximate model, with good spectral properties (in the linear case). In the particular case where a polynomial basis is chosen

for the approximation space, the derived pseudospectral method may be viewed as a collocation method where the collocation points are the zeros of the chosen polynomial. In this case, the reduced model is moreover stated in "natural" variables (the infinite dimensional state variables evaluated at the spatial discretization points), making its physical meaning easy to catch. These collocation (polynomial) methods are the most used in process engineering, specially since the book [22], either for processes simulation or control. Indeed the nice properties of collocation methods make them also very effective to develop control laws on the reduced model (see for instance [23] for input-output linearization, [24] for backstepping or [25] for robust optimal control).

Among the drawbacks of pseudospectral polynomial methods is the difficulty of choosing the numerical parameters which greatly affect dynamical properties of the reduced model. This "choice" problem has been studied in some detail in [26] where a methodology to choose the numerical value of the parameters in polynomial collocation methods is proposed in order to obtain dynamical stability and good numerical conditioning and accuracy. Another drawback of pseudospectral methods is that they result in low order but "full" state space realization of the reduced model, contrarily to, for instance, finite difference or finite elements methods which result in sparse structure matrices. It is then very difficult to exhibit any structural property as geometric structure or invariant (first integrals) in the reduced model. Moreover, without any additional precautions, the polynomial collocation scheme does not preserve dynamical stability of the actual PDE model, neither its energetic properties (energy conservation, dissipativeness) and it introduces noticeable numerical dissipation [21].

In this paper, we aim at developing a polynomial pseudospectral method which preserves some geometric interconnection structure of our model (namely the Dirac structure, see section 2 and [27]), phenomenological laws which come from thermodynamical considerations and general conservation laws without introducing any uncontrolled numerical dissipation. Doing so, we expect nice structural dynamical properties for the obtained reduced model as well as easy implementation of passivity based or energy shaping control techniques. Mixed finite elements methods may be viewed as a particular case of the methodology developed hereafter for the case of low order polynomial approximations. In this sense, this work is a generalization of previous ones [8, 20, 21] and it provides a wider and more theoretical interpretation of implicit choices made in these earlier works. Among these choices, those related to the kernel of exact exterior derivation in exterior differential forms spaces, and to the implicit choice of boundary port variables, as well as their relation with the geometric interconnection structure and its associated power product, will be given in some detail.

The paper is organized as follows : section 2 is dedicated to recalls on the Hamiltonian formulation of open distributed parameter systems, on its key Stokes-Dirac interconnection structure and on illustrative parabolic and hyperbolic examples. The main idea of the reduction scheme we propose, that is performing exact differentiation by choosing several approximation spaces, is defined in section 3. In section 4, the obtained finite dimensional geometric (Dirac) structure is defined using new reduced variables obtained by projection. The kernel and image representation of this structure as well as the choice of (implicit) boundary port-variables are discussed and related to previous works on boundary control systems. The discretization of phenomenological laws which are closure equations for the interconnection structure is discussed in section 5. The examples of section 2 are reduced with the proposed scheme and their power balance equations are written down. In section 6 it is shown on the transmission line example that, while preserving the geometric interconnection structure and invariant (energy) of the actual PDE model, the proposed method also share the excellent spectral behaviour of the classical collocation method.

2 Port-based model for distributed parameter systems

2.1 Dirac interconnection structure

The Dirac structure is a geometric structure introduced originally to gauge Poisson brackets for system with constraints [28]. It has also be used to model power conserving interconnections for open physical systems [7]. Thus, the Dirac structure appears as a generalization of the Poisson structure which one finds usually in classical Hamiltonian systems [1, 28]. Let us recall the mathematical definition of a Dirac structure [7].

Definition 1 (Dirac structure) *Let $\mathscr{F}$ (*flow variables*) and $\mathscr{E}$ (*effort variables*) be two real vectors spaces endowed with the non degenerate bilinear form (*power pairing*) $\langle\cdot,\cdot\rangle : \mathscr{B} = \mathscr{F} \times \mathscr{E} \to \mathbb{R}$. One can define an associated* symmetric *bilinear form by symmetrization on the previous one : $\ll\cdot,\cdot\gg: \mathscr{B}\times\mathscr{B}\to\mathbb{R} : ((f_1,e_1),(f_2,e_2)) \mapsto \ll (f_1,e_1),(f_2,e_2)\gg := \langle e_1|f_2\rangle + \langle e_2|f_1\rangle$. Then the sub-space $\mathscr{D}\subset\mathscr{B}$ is a Dirac structure with respect to the bilinear form $\ll . \gg$ if and only if $\mathscr{D} = \mathscr{D}^{\perp}$, where the orthogonality is defined with respect to the bilinear form $\ll\cdot,\cdot\gg$.*

The flow variables $f \in \mathscr{F}$ and the effort variables $e \in \mathscr{E}$ are said conjugate variables in the sense that their product may be computed with the power pairing $\langle\cdot,\cdot\rangle$.

Definition 2 (Tellegen structure) *The Tellegen interconnection structures, well known from the Tellegen interconnection theorem in circuit theory, may be formalized in a similar way as a "generalization" of Dirac interconnection structures in the bond space [30].*

Let $\mathscr{Z}$ be a sub-space of the bond space $\mathscr{B} = \mathscr{F} \times \mathscr{E}$. Then $\mathscr{Z}$ is called a Tellegen structure if and only if $\mathscr{Z} \subset \mathscr{Z}^{\perp}$ with respect to the bilinear form $\ll . \gg$.

2.2 Stokes-Dirac structure

In this paper we consider a particular case of Dirac structures, the one when the variables are defined on space of differential forms [3]. In this case, the associated power-pairing $\langle \cdot, \cdot \rangle$ is defined using the Stokes theorem modelling the power balance in the system

$$\langle f, e \rangle = \int_Z e \wedge f + \int_{\partial Z} f_\partial \wedge e_\partial \tag{1}$$

where Z is some smooth bounded domain and ∂Z its boundary. In this work, we are interested in the 1D spatial domain $[0, L]$, with its $\{0, L\}$ two-points boundary. Thus, efforts and flux variables belong respectively to 0-forms Λ^0 and 1-forms Λ^1 spaces. For general definition of Stokes-Dirac structure in N-dimensional space, we refer to [7].

Proposition 1 *Let $\mathscr{F}$, $\mathscr{E}$ be respectively the spaces of fluxes and efforts variables. Let $(f^q, f^p; f_\partial) \in \Lambda^1 \times \Lambda^1 \times \mathbb{R}^2 = \mathscr{F}$ and $(e^q, e^p; e_\partial) \in \Lambda^0 \times \Lambda^0 \times \mathbb{R}^2 = \mathscr{E}$. The subspace $\mathscr{D} = (e^q, e^p, f^q, f^p, e_\partial, f_\partial)$ satisfying*

$$\begin{cases} \begin{pmatrix} f^p \\ f^q \end{pmatrix} = \begin{pmatrix} 0 & d \\ d & 0 \end{pmatrix} \begin{pmatrix} e^p \\ e^q \end{pmatrix} & (2) \\ \begin{pmatrix} f_\partial \\ e_\partial \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} e^p|_{\partial Z} \\ e^q|_{\partial Z} \end{pmatrix} & (3) \end{cases}$$

where d denotes the exterior derivative, is a Stokes-Dirac structure (i.e. $\mathscr{D} = \mathscr{D}^{\perp}$) with respect to the symmetric pairing

$$\begin{aligned} &\langle\langle (f_1^p, f_1^q, f_{\partial,1}, e_1^p, e_1^q, e_{\partial,1}), (f_2^p, f_2^q, f_{\partial,2}, e_2^p, e_2^q, e_{\partial,2}) \rangle\rangle = \\ &\qquad \int_Z (e_1^p \wedge f_2^p + e_1^q \wedge f_2^q + e_2^p \wedge f_1^p + e_2^q \wedge f_1^q) + \int_{\partial Z} (e_{\partial,1} \wedge f_{\partial,2} + e_{\partial,2} \wedge f_{\partial,1}) \end{aligned} \tag{4}$$

Proof 1 *See [7] for a proof. Let us now examine two examples (hyperbolic and parabolic) to illustrate the generality of approaches based on such Dirac structure interconnections.*

2.3 An hyperbolic example : the transmission line model

A system $\{\dot{p}, \dot{q}, \delta_p H(q,p), \delta_q H(q,p)\} \in \mathscr{D}$ is called a *port-Hamiltonian system*, with $H(q,p)$ its Hamiltonian or "energy" density depending on the extensive state "energy" variables q and p. Let us recall as an illustration the transmission line model in a port-Hamiltonian form and highlight its underlying Dirac structure. This example is developed in [8]. For simplicity we consider a transmission line without dissipation defined on the 1D spatial domain $[0, L]$. We start from the classical wave equations :

$$\frac{\partial q(t,z)}{\partial t} = -\frac{\partial I(t,z)}{\partial z}, \qquad \frac{\partial p(t,z)}{\partial t} = -\frac{\partial V(t,z)}{\partial z} \tag{5}$$

where $q(t,z)$, $p(t,z)$, $I(t,z)$ and $V(t,z)$ denote respectively the charge density, the flux density, the current and the voltage. Using the following identification

- $e^q = -I$, $e^p = -V$ $\quad e^q, e^p \in \Lambda^0$
- $f^q = \dot{q}$, $\quad f^p = \dot{p}$, $\quad f^p, f^q \in \Lambda^1$

The port-Hamiltonian representation of the equations (5) is then given by:

$$\begin{aligned} f^q &= de^p \\ f^p &= de^q \end{aligned} \tag{6}$$

with the associated boundary variables

$$\begin{aligned} e_\partial^0 &= e^q(0) \qquad & e_\partial^L &= e^q(L) \\ f_\partial^0 &= e^p(0) \qquad & f_\partial^L &= e^p(L) \end{aligned} \tag{7}$$

Thus, we can recognize the Dirac structure defined in proposition 1 above. The port-Hamiltonian model of such transmission lines are completed by adding the Hamiltonian function

$$H = H^c + H^p = \int_0^L \frac{\star q(z)}{2C(z)} \wedge q(z) + \int_0^L \frac{\star p(z)}{2L(z)} \wedge p(z)$$

where $\star$ denotes the Hodge star operator.

2.4 A Parabolic example : the adsorption column model

The model for the adsorption-diffusion of gaseous particles in granular substrates is developed in [20]. This diffusion process provides and example of parabolic system and allows us to show how to apply Dirac structure interconnections also to such parabolic examples. For simplicity, we consider a spherical domain (crystal) with a spherical symmetry of the adsorption process. Thus our model again reduces to a distributed parameters system defined on a 1D spatial problem $[0,L]$. The Stefan-Maxwell model for diffusion yields the following equations [31]

$$N^{ads} = -\frac{\star qD}{RT} \wedge d\mu^{ads} \tag{8}$$

where $\mu^{ads} \in \Lambda^0$ is the adsorbed particles chemical potential in the mixing, $N^{ads} \in \Lambda^1$ the molar flux of adsorbed particles, $q \in \Lambda^1$ the molar concentration, D the Stefan-Maxwell diffusivity, R the perfect gas constant, and T the temperature. The balance equation for adsorbed particles (conservation law) is then :

$$\dot{q} = -dN^{ads} \tag{9}$$

These two relations are augmented with a closure relation which derives from the first principle and expresses the chemical potential μ^{ads} as a variational derivative of the internal energy with respect to variations of the molar concentration q. If a Langmuir constitutive relation is chosen for the internal energy dependance to the concentration q, this may be expressed as:

$$\mu = \mu^0(T,P) + RTln\Big(\frac{\star q}{\star q^{sat}}\Big) \tag{10}$$

where q^{sat} denotes the saturation concentration, P the pressure and μ^0 the reference chemical potential. Considering the following identifications

- $e^q = \mu, \;\; e^p = -N^{ads} \quad e^q, e^p \in \Lambda^0$
- $f^q = \dot{q}, \;\; f^p = de^q, \quad f^p, f^q \in \Lambda^1$

we recognize again the Dirac structure in 1. To obtain a complete model formulation, one has to augment this structure with the two closure constitutive relations (8) and (10).

3 A polynomial geometric discretization scheme

In the previous section we have seen how Stokes-Dirac interconnection structures may be used to model both hyperbolic and parabolic simple distributed parameters systems. This interconnection structure both guarantees power conservation (and resulting energy balance equations) and completely specifies the way every model subparts interact together. This is the reason why we build the spatial reduction scheme presented in this section on the discretization of the Stokes-Dirac structure. The scheme is based on the use of polynomial pseudo-spectral methods restricted in order to guarantee the "conservation" of the interconnection structure. Note that such approaches have already been developed but only on linear mixed finite elements methods (see [19, 8, 20]). Our purpose is to generalize these works to pseudo-spectral methods in general, to develop a systematic way to deduce the resulting finite Dirac structure, to interpret this structure in term of a reduced power product, and to connect these results to implicit choices of boundary conditions and boundary control systems. We will use, for the spatial reduction, polynomial approximation bases (with Lagrange interpolation) in such a way that the reduced variables will be approximations of the distributed ones at chosen "collocation" points. Usually these points are zeros of orthogonal polynomials in order to to reduce the solution oscillations. A methodology to select them, according to conditioning and dynamical stability of the reduced system, is presented in [26].

3.1 Polynomial approximation and exact differentiation

The effort variables are approximated in 0-forms polynomial base, when the flux variables are approximated in 1-forms one, in accordance with the infinite dimensional case. Hence we define the approximations :

$$e^q(z) = \sum_{i=0}^{N} e_i^q \varphi_i(z) \tag{11}$$

$$e^p(z) = \sum_{i=0}^{N} e_i^p \varphi_i(z) \tag{12}$$

$$f^q(z) = \sum_{i=0}^{N-1} f_i^q \psi_i(z)dz \tag{13}$$

$$f^p(z) = \sum_{i=0}^{N-1} f_i^p \psi_i(z)dz \tag{14}$$

where $\varphi_i(z)$ and $\psi_i(z)$ are interpolating Lagrange polynomials, respectively of degree N and $N-1$ defined as

$$\varphi_i(z) = \prod_{j=0, j\neq i}^{N}, \frac{z-\zeta_j}{\zeta_i-\zeta_j} \quad \psi_i(z) = \prod_{k=0, k\neq i}^{N-1} \frac{z-z_k}{z_i-z_k}$$

satisfying $\varphi_i(\zeta_j) = \delta_{ij}$ and $\psi_i(z_j) = \delta_{ij}$, ζ_j, $j = 0,...,N$ being the interpolating points associated to the φ_j base, while z_j, $j = 0,...,N-1$ are those of the ψ base.
Inserting relations (11) - (14) into (2), and evaluating the approximations at the collocation points z_k (zeros of the ψ_i Lagrange polynomials). Finally we get the following matrix relations:

$$\begin{aligned} f_k^q &= \sum_{i=0}^{N} D_{k,i} e_i^p \\ f_k^p &= \sum_{i=0}^{N} D_{k,i} e_i^q \end{aligned} \tag{15}$$

where D is a $N \times (N+1)$ matrix obtained by exact differentiation

$$D_{k,i} = \frac{d\varphi_i}{dz}(z_k)$$

The boundary variables are defined according to (3) by polynomial interpolation of efforts e^p, e^q (0-forms) in the two-boundary points 0 and L.

$$\begin{aligned} e_\partial^0 &= e^q(0) = \sum_{i=0}^{N} e_i^q \varphi_i(0) \\ e_\partial^L &= e^q(L) = \sum_{i=0}^{N} e_i^q \varphi_i(L) \\ f_\partial^0 &= e^p(0) = \sum_{i=0}^{N} e_i^p \varphi_i(0) \\ f_\partial^L &= e^p(L) = \sum_{i=0}^{N} e_i^p \varphi_i(L) \end{aligned} \tag{16}$$

Relations (15) and (16) can be written in matrix form

$$\begin{pmatrix} e_\partial^0 \\ e_\partial^L \\ f_\partial^0 \\ f_\partial^L \\ f^q \\ f^p \end{pmatrix} = \begin{pmatrix} \varphi(0)^T & 0 \\ \varphi(L)^T & 0 \\ 0 & \varphi(0)^T \\ 0 & \varphi(L)^T \\ 0 & D \\ D & 0 \end{pmatrix} \begin{pmatrix} e^q \\ \\ e^p \end{pmatrix} \tag{17}$$

where $e_\partial^0, e_\partial^L, f_\partial^0, f_\partial^L \in \mathbb{R}$, and f^q, f^p are $\mathbb{R}^N$ functions while e^q, e^p are $\mathbb{R}^{N+1}$ functions. The vectors $\varphi(0)^T$ and $\varphi(L)^T$ being the vectors of polynomials $\varphi_i(z)$ evaluated respectively at the boundary points $z = 0$ and $z = L$.

3.2 Power product, Stokes Theorem and reduced Tellegen structure

Replacing the flux and effort variables e_i^q, e_i^p, f_i^q, f_i^p, $i = 1,2$ by their approximations in (4), the discretization of the symmetric power product gives

$$\begin{pmatrix} e_1^p \\ e_1^q \\ e_1^0 \\ e_1^L \\ f_1^p \\ f_1^q \\ f_1^0 \\ f_1^L \end{pmatrix}^T \begin{pmatrix} 0 & 0 & 0 & 0 & M & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & M & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ M^T & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & M^T & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} e_2^p \\ e_2^q \\ e_2^0 \\ e_2^L \\ f_2^p \\ f_2^q \\ f_2^0 \\ f_2^L \end{pmatrix} \tag{18}$$

where M is the $(N+1) \times N$ matrix whose elements are

$$M_{i,j} = \int_0^L \varphi_i(z) \psi_j(z) dz \tag{19}$$

It's important to notice that M^T has a non-zero kernel $Ker(M^T) \subset \mathscr{E}$ due to the fact that the "differentiation" map is not injective (neither is the exterior derivative in the infinite dimensional case). As a consequence, the symmetric pairing (18) is degenerate. This is an obstruction to the definition of a Dirac structure with respect to this pairing. However one may extend the definition of the Tellegen structure given in the definition 2 on bond spaces endowed with a *degenerate* pairing such as (18).

Proposition 2 *Let $\mathscr{B} = \mathscr{F} \times \mathscr{E} = \mathbb{R}^{2N+2} \times \mathbb{R}^{2N+4}$ be the reduced finite dimensional bond space. Then, the subspace $\mathscr{D} = (f^p, f^q, f^0_\partial, f^L_\partial, e^p, e^q, e^0_\partial, e^L_\partial) \subset \mathscr{B}$ of port-variables satisfying relation (17) is a Tellegen structure with respect to the symmetric power product (18).*

Proof 2 *Let $(f^p_1, f^q_1, f^0_{\partial 1}, f^L_{\partial 1}, e^p_1, e^q_1, e^0_{\partial 1}, e^L_{\partial 1}), (f^p_2, f^q_2, f^0_{\partial 2}, f^L_{\partial 2} e^p_2, e^q_2, e^0_{\partial 2}, e^L_{\partial 2}) \in \mathscr{B}$ Developing the symmetric product in (18), replacing the M matrix by its expression in (19) first, and the discrete effort and flux variables by their expressions in (15), it is easy to check that the symmetric product (18) can be written*

$$\int_0^L e^p_1(z)de^q_2(z) + e^q_1(z)de^p_2(z) + e^p_2(z)de^q_1(z) + e^q_2(z)de^p_1(z) - e^0_{\partial 1}f^0_{\partial 2} + e^L_{\partial 1}f^L_{\partial 2} - f^0_{\partial 1}e^0_{\partial 2} + f^L_{\partial 1}e^L_{\partial 2}$$
$$= -\int_0^L d(e^p_1(z)e^q_2(z)) + d(e^q_1(z)e^p_2(z)) - e^0_{\partial 1}f^0_{\partial 2} + e^L_{\partial 1}f^L_{\partial 2} - f^0_{\partial 1}e^0_{\partial 2} + f^L_{\partial 1}e^L_{\partial 2} = 0$$

As a consequence of the Stokes theorem which comes down to simple integration by parts in this 1D case.

4 Discretized Dirac structure on a reduced bond space

4.1 Dirac structure as a quotient of the Tellegen's structure

The existence of a Tellegen structure $\mathscr{D}$ in the bond space $\mathscr{B}$ suggests the existence of some "restricted" Dirac structure $\mathscr{D}_r$. This is related to the fact that the symmetric bilinear form (18) used to define the Tellegen structure $\mathscr{D}$ is degenerate

$$Ker(\ll \cdot, \cdot \gg) = 0_{\mathscr{F}} \times 0_{\mathscr{F}} \times Ker(M^T) \times Ker(M^T)$$

Hence the Dirac structure will be obtained from the quotient of Tellegen structure by the kernel of M^T .

4.2 Image representation of the finite Dirac structure

We will now derive a representation of the Dirac structure from the symmetric power product (18), and in so doing we prove its existence. First, let us give a useful representation of a Dirac structure in the general finite dimensional case.

Definition 3 *Let $\mathscr{D} \subset \mathscr{F} \times \mathscr{E}$, with $dim\mathscr{F} = dim\mathscr{E} = n$, and σ some signature diagonal matrix associated with the pairing (18), $\sigma = \{1, 1, -1, 1\}$. Any two $n \times n$ matrices, denoted here E and F, and satisfying*

1. $E\sigma F^T + F\sigma E^T = 0$
2. $rank[E : F] = n$

define a Dirac structure $\mathscr{D} = \{(f, e) \in \mathscr{F} \times \mathscr{E} | f = E^T\lambda, e = F^T\lambda,\ \lambda \in \mathbb{R}^n\}$ associated with the bilinear symmetrization of the canonic power pairing in $\mathscr{F} \times \mathscr{E}$. This description is called an image representation *of the Dirac structure $\mathscr{D}$ [2, 5].*

We will now find the two matrices E and F satisfying these two axioms for the reduced Dirac structure $\mathscr{D}$ obtained by the polynomial approximation scheme defined above. First we use the Tellegen structure of the reduced system to conclude to the vanishing of the symmetric power product (18). Hence

$$e^{pT}_1 M f^p_2 + e^{qT}_1 M f^q_2 + f^{pT}_1 M^T e^p_2 + f^{qT}_1 M^T e^q_2 - e^0_{\partial 1}f^0_{\partial 2} + e^L_{\partial 1}f^L_{\partial 2} - f^0_{\partial 1}e^0_{\partial 2} + f^L_{\partial 1}e^L_{\partial 2} = 0 \tag{20}$$

Replacing the flux and effort variables in (20) by their expressions in from the reduced Dirac structure (17), one gets

$$e^q_1(MD + D^TM^T - T^0 + T^L)e^p_2 + e^p_1(MD + D^TM^T - T^0 + T^L)e^q_2 = 0 \tag{21}$$

where T^0 is the $(N+1) \times (N+1)$ matrix with elements $T^0_{ij} = \varphi_i(0)\varphi_j(0)$, and T^L the $(N+1) \times (N+1)$ matrix with elements $T^L_{ij} = \varphi_i(L)\varphi_j(L)$. Since (21) holds for any (e^q_1, e^p_2) and for any (e^p_1, e^q_2), we deduce

$$MD + D^TM^T - T^0 + T^L = 0 \tag{22}$$

This result which may be seen as the "finite-dimensional" Stokes theorem, will be very useful for the sequel.

Remark 1 *If $T^L - T^0 = 0$ in (22), which is the case for isolated system without any energy exchange across its boundaries, we get $MD + D^T M^T = 0$. The matrix MD is thus skew-symmetric and we can recognize a well-known a Poisson structure for conservative systems.*

According to (17) we can write

$$\begin{pmatrix} f^q \\ f^p \\ f^0_\partial \\ f^L_\partial \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & D \\ D & 0 \\ 0 & \varphi(0)^T \\ 0 & \varphi(L)^T \end{pmatrix}}_{E^T} \begin{pmatrix} e^q \\ e^p \end{pmatrix} \tag{23}$$

where f^q and f^p are in $\mathbb{R}^N$ while e^q and e^p are $\mathbb{R}^{N+1}$. In addition, we introduce the projected efforts $\tilde{e}^q$, $\tilde{e}^p \in \mathbb{R}^N$ defined as

$$\begin{aligned} \tilde{e}^q &= M^T e^q \\ \tilde{e}^p &= M^T e^p \end{aligned} \tag{24}$$

These projected efforts allow to complete the image representation of the reduced Dirac structure $\mathscr{D}_r$. According to (24) and (17), one has

$$\begin{pmatrix} \tilde{e}^q \\ \tilde{e}^p \\ e^0_\partial \\ e^L_\partial \end{pmatrix} = \underbrace{\begin{pmatrix} M^T & 0 \\ 0 & M^T \\ \varphi(0)^T & 0 \\ \varphi(L)^T & 0 \end{pmatrix}}_{F^T} \begin{pmatrix} e^q \\ e^p \end{pmatrix} \tag{25}$$

Proposition 3 *The sub-space*

$$\mathscr{D}_r = \left\{ \left(E^T\lambda, F^T\lambda\right) \middle| \lambda \in \mathbb{R}^{2N+2} \right\}$$

is a Dirac structure in $\mathscr{F} \times \mathscr{E} = \mathbb{R}^{2N+2} \times \mathbb{R}^{2n+2}$. This representation is called image representation [2, 5].

Proof 3 *(*i*)* $E\sigma F^T + F\sigma E^T = 0$

$$\begin{aligned} E\sigma F^T + F\sigma E^T = &\begin{pmatrix} 0 & D^T & 0 & 0 \\ D^T & 0 & \varphi(0) & \varphi(L) \end{pmatrix} \times \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} M^T & 0 \\ 0 & M^T \\ \varphi(0)^T & 0 \\ \varphi(L)^T & 0 \end{pmatrix} \\ &+ \begin{pmatrix} M & 0 & \varphi(0) & \varphi(L) \\ 0 & M & 0 & 0 \end{pmatrix} \times \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & D \\ D & 0 \\ 0 & \varphi(0)^T \\ 0 & \varphi(L)^T \end{pmatrix} \end{aligned} \tag{26}$$

After elementary calculation (26) gives

$$\begin{pmatrix} 0 & D^T M^T + MD - T^0 + T^L \\ D^T M^T + MD - T^0 + T^L & 0 \end{pmatrix} \tag{27}$$

According to (22) we get $E\sigma F^T + F\sigma E^T = 0$

*(*ii*)* $[E : F]$ *is full rank* $(2n+2)$

We should show that $(D_1^T, D_2^T, ..., D_n^T, \varphi(0))$ is an independent set. where $D_i^T = \varphi(z_i)$ the N column vectors of $(N+1) \times N$ D^T matrix, the z_i, $i = 1, 2, ..., N$ are the N interpolating points of ψ polynomial base.

We prove it by contradiction. Let assume that the set under consideration is dependent. This supposes one can deduce $\varphi(0)$, and thus a polynomial set of degree N, and that only with N z_i points. Actually,

$$\varphi(z) = \alpha_0 \varphi(0) + \int_0^z \sum_{i=1}^{N} \alpha_i \varphi_i'(z) dz$$

But it is known that one cannot generate polynomial of degree N with only N interpolating points, which contradicts our assumption, so $(\varphi'(z_1), \varphi'(z_2), ..., \varphi(0))$ is an independent and maximal set in $\mathbb{R}^{n+1}$ therefore it is a base. Thus,

$$\begin{pmatrix} D^T & \varphi(0) & 0 & 0 \\ 0 & 0 & D^T & \varphi(0) \end{pmatrix} \tag{28}$$

is an independent and maximal set in $\mathbb{R}^{2n+2}$ and thus, concatenate matrix $[E : F]$ is full rank, $2n+2$.

These two results suggest the existence of some skew-symmetric and full rank matrix J relating effort and flux variables

$$\begin{pmatrix} f^q \\ f^L_\partial \\ f^p \\ -e^0_\partial \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & \begin{pmatrix} D \\ \varphi(L) \end{pmatrix} \begin{pmatrix} M^T \\ \varphi(0) \end{pmatrix}^{-1} \\ \begin{pmatrix} D \\ -\varphi(0) \end{pmatrix} \begin{pmatrix} M^T \\ \varphi(L) \end{pmatrix}^{-1} & 0 \end{pmatrix}}_{J} \begin{pmatrix} \tilde{e}^q \\ e^L_\partial \\ \tilde{e}^p \\ f^0_\partial \end{pmatrix} \tag{29}$$

This representation is called the *input output representation*, see [30]. We can check easily that the matrix J is skew-symmetric. Actually, calculating the anti-diagonal element's sum

$$\begin{pmatrix} D \\ \varphi(L) \end{pmatrix} \begin{pmatrix} M^T \\ \varphi(0) \end{pmatrix}^{-1} + \left(\begin{pmatrix} D \\ -\varphi(0) \end{pmatrix} \begin{pmatrix} M^T \\ \varphi(L) \end{pmatrix}^{-1} \right)^T = \left(M\varphi(L)^T\right)^{-1} \left(MD + D^T M^T - T^0 + T^L\right) \begin{pmatrix} M^T \\ \varphi(0) \end{pmatrix}^{-1} = 0 \tag{30}$$

according to (22).

Remark 2 *Actually the input output representation (29) is a particular of choice of inputs and outputs. It may be generalized by choosing as input and output variables any linear combinations of the boundary port variables defined in (23) and (25):*

$$\begin{pmatrix} u \\ y \end{pmatrix} = \begin{pmatrix} W \\ \tilde{W} \end{pmatrix} \begin{pmatrix} f_\partial \\ e_\partial \end{pmatrix} \tag{31}$$

The definition of the matrices W and $\tilde{W}$ is not further dicussed here but may be related to the definition of boundary control systems associated with the port Hamiltonian systems defined on Stokes Dirac structures in [32].

5 Discretization of the constitutive relations

In previous sections we have presented a discretization approach preserving the geometric Dirac structure of the original model. We have seen that this structure is common to both transmission line and adsorption-diffusion models. In this section, we will apply this reduction scheme to the discretization of conservative and dissipative closure equations in order to derive finite dimensional closure equations of the same *energetic kind*. The basic idea is thus to approximate the stored energy or the dissipated power in the previously chosen approximation spaces.

5.1 Transmission line constitutive relations

In the transmission line example only conservative constitutive phenomena are considered. The needed closure relations are obtained from the Hamiltonian expression

$$H = H^q + H^p = \int_0^L \frac{\star q(z,t)}{2C(z)} q(z,t) + \frac{\star p(z,t)}{2L(z)} p(z,t) \tag{32}$$

This leads to the corresponding power expression

$$\frac{dH}{dt} = \int_0^L \frac{\star q(z,t)}{C(z)} \dot{q}(z,t) + \frac{\star p(z,t)}{L(z)} \dot{p}(z,t) \tag{33}$$

which could be identified with the global expression giving a Hamiltonian system power, see [7]

$$\frac{dH}{dt} = \int_Z \delta_q H \wedge \dot{q} + \delta_p H \wedge \dot{p} = \int_Z e^q \wedge f^q + e^p \wedge f^p \tag{34}$$

The Hamiltonian $H(p,q)$ depends on the 1-forms p and q. They are approximated using the ψ polynomial base as in section 3

$$\begin{aligned} q(z,t) &= \sum_{i=0}^{N-1} q_i(t)\psi_i(z)dz \\ p(z,t) &= \sum_{i=0}^{N-1} p_i(t)\psi_i(z)dz \end{aligned} \tag{35}$$

Inserting (35) into (33) the approximate power can be written

$$\frac{dH}{dt} = q^T(t)C\dot{q}(t) + p^T(t)L\dot{p}(t) \tag{36}$$

where

$$C_{ij} = \int_0^L \frac{\psi_i(z)\psi_j(z)}{C(z)} dz$$

and

$$L_{ij} = \int_0^L \frac{\psi_i(z)\psi_j(z)}{L(z)} dz$$

In addition we know that the Hamiltonian takes the form

$$\frac{d\bar{H}}{dt} = \sum_{i=0}^{N-1} \frac{\partial \bar{H}}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial \bar{H}}{\partial p_i}\frac{dp_i}{dt} \tag{37}$$

Identifying (37) with (36) we get the approximate efforts expressions

$$\begin{aligned} e_i^q(t) &= \sum_{j=0}^{N} C_{ij} q_j(t) \\ e_i^p(t) &= \sum_{j=0}^{N} L_{ij} p_j(t) \end{aligned} \tag{38}$$

The discretized flux are deduced from efforts using the structure relation (29). This solves the whole problem of the wave equation.

5.2 Adsorption-diffusion constitutive relations

In the adsorption-diffusion example both conservative and dissipative constitutive phenomena are considered. Two closure relations are needed to complete the model, the first one deriving from the expression of the stored chemical energy, and the other from the diffusion model.

5.2.1 Discretization of the chemical stored energy

The Langmuir relation (10) has been chosen to describe the dependance of the internal energy to the species concentration $q(t,z)$. Let H denotes this total chemical energy. Then

$$\begin{aligned} \frac{dH}{dt} &= \int_0^L f^q(t,z) \wedge e^q(t,z) \\ &= \int_0^L \dot{q}(t,z) \wedge \mu(q) \\ &= \int_0^L \dot{q}(z,t) \wedge \left(\mu^0(P,T) + RT\, ln(\frac{\star q}{\star q^{sat}}) \right) \end{aligned} \tag{39}$$

The density q being a 1-form, this power is approximated using the ψ polynomial base

$$q(t,z) = \sum_{i=0}^{N-1} q_i(t)\psi_i(z) dz \tag{40}$$

Inserting (40) into (39) we get

$$\frac{dH}{dt} = \sum_{i=0}^{N-1} \dot{q}_i \int_0^L (\mu^0 + RT \ln \frac{\sum_{j=0}^{N-1} q_j \psi_j(z)}{q^{sat}}) \psi_i(z) dz = \sum_{i=0}^{N-1} \dot{q}_i(t) e_i^q(t) \tag{41}$$

where the approximated efforts e_i^q are defined as in a generic capacitive element by

$$e_i^q(t) = \int_0^L (\mu^0 + RT \ln(\frac{\sum_j q_j(t)\psi_j(z)}{q^{sat}})) \psi_i(z) dz \tag{42}$$

5.2.2 Discretization of diffusion relation

The discretization of the diffusion may be obtained writing the dissipative power P

$$P = \int_0^L -N^{ads} \wedge d\mu = \int_0^L f^p(t,z) \wedge e^p(t,z) \tag{43}$$

with

$$e^p(t,z) = -\frac{D \star q(t,z)}{RT} f^p(t,z)$$

Since f^p is a 1-form we can approximate it as

$$f^p(t,z) = \sum_{i=0}^{N-1} f_i^p(t)\psi_i(z)dz \tag{44}$$

The approximate power may then be written

$$P = \sum_{i,j,k=0}^{N-1} f_i^p(t)\left(\frac{D}{RT}q_j(t)f_k^p(t)\int_0^L \psi_i\psi_j\psi_k dz\right) = \sum_{i=0}^{N-1} f_i^p(t)e_i^p(t) \tag{45}$$

with $e_i^p(t)$ defined as

$$e_i^p(t) = \sum_{j,k=0}^{N-1} \frac{D}{RT}q_j(t)f_k^p(t)\int_0^L \psi_i\psi_j\psi_k dz \tag{46}$$

Discretized constitutive equations (42) and (46) complete the reduced Dirac structure equations for the adsorption-diffusion model and provide a "ready to integrate" reduced port-based model of ordinary differential equations.

6 Numerical example

Consider a simple line transmission with constant parameter (inductance I=2, capacitance C=3 and resistance R=0). In this particular case, the resulting PDE is linear. Thus, we can formally compute the model dynamical spectrum from the underlying eigenvalue problem and compare it with the spectrum of the finite dimensional model obtained using the discretization scheme developed in this paper. symmetric Dirichlet boundary conditions $q(0) = 0$ and $p(L) = 0$ have been chosen to complete the ideal transmission line model written in the form :

$$\begin{pmatrix} 0 & d \\ d & 0 \end{pmatrix}\begin{pmatrix} \frac{q(z)}{C} \\ \frac{p(z)}{L} \end{pmatrix} = \lambda \begin{pmatrix} q \\ p \end{pmatrix} \tag{47}$$

The values in table 1 and 2 below compare the "exact" eigenvalues of this ideal transmission line example and those obtained for the two reduced models obtained by the "classical" collocation method and the geometric collocation method we propose in this paper. In table 1, 8 interior collocation points have been chosen and the 8 resulting pairs of imaginary eigenvalues are reported. In table 2, 16 interior collocation points have been chosen but only the 8 first pairs of eigenvalues are listed. To achieve the symmetric Dirichlet boundary conditions, the chosen polynomial bases have been augmented (in the "classical collocation" case) by considering the developments

$$q(z) = \sum_{i=1}^{8} q_i\psi_i(z)z, \qquad p(z) = \sum_{i=1}^{8} p_i\psi_i(z)(z-L) \tag{48}$$

which automatically satisfy $q(0) = 0$ and $p(L) = 0$. The eigenvalues of the model resulting from our "geometric" collocation method are obtained by the diagonalization of the matrix $J \times Q$ from the input-output representation (29) when substituting the efforts from (38) and again considering Dirichlet conditions $q(0) = 0$ and $p(L) = 0$. One obtains

$$\begin{pmatrix} f^q \\ f_\partial^L \\ f^p \\ e_\partial^0 \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & \begin{pmatrix} D \\ \varphi(L) \end{pmatrix}\begin{pmatrix} M^T \\ \varphi(0) \end{pmatrix}^{-1} \\ \begin{pmatrix} D \\ -\varphi(0) \end{pmatrix}\begin{pmatrix} M^T \\ \varphi(L) \end{pmatrix}^{-1} & 0 \end{pmatrix}\begin{pmatrix} C & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & L & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}}_{J\times Q}\begin{pmatrix} q \\ e_\partial^L \\ p \\ f_\partial^0 \end{pmatrix} \tag{49}$$

In the first case (8 interior collocation points) the geometric method spectrum approximation is more accurate than the classical one with a 10^5 order of magnitude when considering the first eigenvalue pair for instance. It has to be noticed than the classical orthogonal collocation method is already a reference method for its high precision spectrum approximation. In both cases the eigenvalues pairs are close to the imaginary axe (they are on the axe at the machine precision). This is automatically the case for the geometric method since the Dirac structure is preserved and thus no numerical dissipation can occur. To understand why this is also the case in this example for the classical collocation method is still an open problem at the moment we are writing this paper. However, in has been noticed in [10] that classical collocation does not preserve the lossless property and introduces significant numerical dissipation in another example (the shallow water model for flow dynamics in reaches which is an hyperbolic transmission model very similar to the transmission line).

Theoretical values	Geometric method	Classical collocation
± 0.32063745754047i	0.00000000000000 ± 0.32063745754047i	0.00000000000000 ± 0.32063745744583i
± 0.96191237262140i	0.00000000000000 ± 0.96191238151097i	0.00000000000000 ± 0.96191420177938i
± 1.60318728770233i	0.00000000000000 ± 1.60321563740732i	0.00000000000000 ± 1.60338416589471i
± 2.24446220278326i	0.00000000000000 ± 2.24771134219675i	0.00000000000000 ± 2.25154046253161i
± 2.88573711786419i	0.00000000000000 ± 2.94830702957369i	0.00000000000000 ± 3.00613251338085i
± 3.52701203294513i	0.00000000000000 ± 3.98374558826630i	0.00000000000000 ± 4.38041246765385i
± 4.16828694802606i	0.00000000000000 ± 6.38606332778657i	0.00000000000000 ± 8.49771153485658i
± 4.80956186310699i	0.00000000000000 ±18.76179259703309i	0.00000000000000 ± 31.96188912930034i

Table 1: Spectrum of an ideal transmission line model: theoretical values (1st column) computed using pseudo-spectral method with 8 interior collocation points. In the 2nd column the corresponding eigenvalues computed using the geometric collocation method. In the 3rd column the eigenvalues obtained by classical collocation.

Theoretical values	Geometric method	Classical collocation
± 0.32063745754047i	0.00000000000000 ± 0.32063745754047i	0.00000000000000 ± 0.32063745754047i
± 0.96191237262140i	0.00000000000000 ± 0.96191237262140i	0.00000000000000 ± 0.96191237262140i
± 1.60318728770233i	0.00000000000000 ± 1.60318728770233i	0.00000000000000 ± 1.60318728771753i
± 2.24446220278326i	0.00000000000000 ± 2.24446220278362i	0.00000000000000 ± 2.24446219878353i
± 2.88573711786419i	0.00000000000000 ± 2.88573711861816i	0.00000000000000 ± 2.88573694719959i
± 3.52701203294513i	0.00000000000000 ± 3.52701228702717i	0.00000000000000 ± 3.52701693319326i
± 4.16828694802606i	0.00000000000000 ± 4.16831018776372i	0.00000000000000 ± 4.16838360476415i
± 4.80956186310699i	0.00000000000000 ± 4.81033320045240i	0.00000000000000 ± 4.81112055125995i

Table 2: Spectrum of an ideal transmission line model: theoretical values (1st column) calculated using pseudo-spectral method with 16 collocation points. In the 2nd column the corresponding eigenvalues calculated using geometric collocation method.In the 3rd column the eigenvalues obtained by classical collocation.

7 CONCLUSIONS AND FUTURE WORKS

In this paper we discussed the geometric discretization of port-based distributed parameters models. We have chosen the transmission line and adsorption-diffusion models as paradigmatic examples of respectively hyperbolic and parabolic systems. We have chosen different approximation spaces according to the degrees of the approximated differential forms. Doing this both the exterior derivative and the boundary operator may be discretized exactly. However one obtains in a first instance a Tellegen structure defined with respect to a degenerate pairing as the dimensions of the spaces of flow and effort variables are not equal. Then a Dirac structure has been obtained as the quotient of the Tellegen structure with respect to the kernel of the degenerate pairing. This Dirac structure is completed with the discretization of the constitutive relations describing either internal energy or irreversible transport phenomena. The resulting reduced model has the structure of a finite-dimensional port hamiltonian system. This port Hamiltonian system form allows the use of passivity-based control laws with the accurate spectral properties that pseudo-spectral methods provide. In view of the many advantages that this method does offer, we are currently extending these results to two dimensional case still within the port-Hamiltonian formalism.

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