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Symplectic spatial integration schemes for systems of balance equations

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ABSTRACT

A method to generate geometric pseudo-spectral spatial discretization schemes for hyperbolic or parabolic partial differential equations is presented. It applies to the spatial discretization of systems of conservation laws with boundary energy flows and/or distributed source terms. The symplecticity of the proposed spatial discretization schemes is defined with respect to the natural power pairing (form) used to define the port-Hamiltonian formulation for the considered systems of balance equations. The method is applied to the resistive diffusion model, a parabolic equation describing the plasma dynamics in tokamaks. A symplectic Galerkin scheme with Bessel conjugated bases is derived from the usual Galerkin method, using the proposed method. Besides the spectral and energetic properties expected from the symplecticity of the method, it is shown that more accurate approximation of eigenfunctions and reduced numerical oscillations result from this choice of conjugated approximation bases. Finally, the obtained numerical results are validated against experimental data from the tokamak Tore Supra facility.

1. Introduction

Hamiltonian operators are classically used to represent the dynamics of many closed systems of conservation laws. Recently port-Hamiltonian (PH) extensions have been introduced to model open systems with boundary or distributed energy flow [29,20]. This modelling approach has proven to be fruitful for the modelling, simulation and control of many hyperbolic systems such as transmission line models [13], beam equations [18] or shallow water equations [15]. However, the same approach may as well be applied to "first principle" parabolic examples such as transport models for adsorption columns [3], fuel cells [11] or diffusion in Ionic Polymer-Metal Composites [23]. Both hyperbolic and parabolic examples make use of a Stokes-Dirac interconnection structure for the realization of the balance equations (e.g. mass, entropy, momentum, etc.).

In the spatial discretization of distributed parameters systems as well as in geometric time integration for ordinary differential equations, pseudo-spectral methods are often chosen because they lead to low order approximate models, with accurate spectral properties (in the linear case, see for instance [10]). Accurate spectral properties and low order models are obviously important features for the design, supervision and control engineering problems. However it is known that key system theoretic properties (both internal or input–output) may be lost in the spatial discretization of distributed parameters systems, when using these pseudo-spectral methods without any additional considerations (as it is also the case for finite-difference schemes). One way of avoiding such problems in the numerical integration of closed Hamiltonian models is to consider geometric methods, i.e. methods which preserve some conserved quantities and/or the geometric interconnection structure of the original model [14]. The latter are usually referred to as symplectic integration methods. The symplecticity is then defined with respect to some Poisson structure. However, these methods usually apply only to the time-integration of closed Hamiltonian systems and not to the spatial discretization of open port-Hamiltonian systems. It must be noticed however that multi-symplectic methods have been developed for the simultaneous space and time integration (i.e. total discretization) of infinite dimensional closed Hamiltonian models [26].

In this paper we define how to systematically build a symplectic spatial discretization scheme for open port-Hamiltonian systems, starting from any given non symplectic pseudo-spectral discretization method (see for instance [9] for a general presentation of classical pseudo-spectral methods). Generalizing previous ideas from [6] (mixed finite elements methods) or [22] (mixed

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orthogonal collocation) we define several approximation bases for the thermodynamical variables, according to their geometric nature (i.e. the degrees of the corresponding differential forms). Then the balance (or conservation) equations and the constitutive (closure) equations are projected into the chosen approximation spaces in order to preserve a power pairing form. The symplecticity of the built mixed pseudo-spectral method is thus defined wit respect to this power pairing form, which acts on the distributed and boundary port variables (i.e. the input–output variables).

A second contribution of the paper is related to the choice of approximation spaces. In the proposed construction of mixed symplectic pseudo-spectral spatial discretization methods, the chosen approximation spaces have to be compatible (conjugated) to guarantee the preservation of the power pairing form. Otherwise they could theoretically be chosen quite freely. Classical choices for the approximation spaces are for instance those spanned by Fourier, wavelets or polynomial bases. Not much has been written however about how to choose practically the approximation space among these many possibilities, in the general case. In this work we suggest the use of approximation spaces spanned by conjugated bases of eigenfunctions associated to a simplified problem, this problem being derived by linearization of the original distributed parameters system and spatial uniformization of its parameters. Besides accurate eigenvalues approximations, such choices also provide accurate accurate eigenfunctions approximations. We show on the considered resistive diffusion example how this choice may solve some numerical oscillation problem encountered with distributed actuation or sharp initial conditions.

To illustrate the approach we have chosen to apply these ideas on the example of the port-Hamiltonian formulation for the 1D resistive diffusion equation [5]. It is a simple plasma control model for the radial diffusion of the poloidal magnetic flux in a tokamak facility. It is a parabolic problem which still may be written in the port-Hamiltonian formalism using a skew symmetric interconnection structure and toric magnetic coordinates with a homogeneous boundary condition at the center (for symmetry) and a non autonomous (controlled) boundary condition at the outer radius. In this example classical (non symplectic) finite difference or collocation spatial discretization schemes give rise to unwanted numerical oscillating (or even unstable) modes. Simulation results obtained with the proposed symplectic reduction scheme have been validated and compared with experimental data obtained from a discharge of the tokamak Tore Supra discharge (this device is described in [21]).

The paper is organized as follows. In Section 2 we recall existing results on the port-Hamiltonian formulation for open distributed parameter systems. In Section 3 we present the proposed methodology to build mixed symplectic spatial discretization schemes, starting from classical pseudo-spectral methods. In Section 4, we derive a mixed Galerkin method for the resistive diffusion problem, using conjugated approximation bases spanned by Bessel's functions. In Section 5.1, we analyze numerical results obtained for the resistive diffusion equation with non-uniform resistivity and distributed non inductive current. These numerical results are also compared against experimental data.

2. Port-based modelling for systems of balance equations with boundary energy flows

Quite recently, an intrinsic formulation of port-based models for distributed parameter systems (described by partial differential state space equations) with boundary energy flow have been proposed [29]. It is based on the definition of the state variables as the densities of some thermodynamical extensive variables. The time derivatives of these variables and their conjugated intensive variables[1] form together the pairs of variables which are used to define a power pairing form and a port-Hamiltonian formulation for systems of conservation laws. Using these variables the usual port Hamiltonian formulation is extended to the infinite-dimensional systems using a canonical geometric interconnection structure called Stokes-Dirac structure [29]. We shall now briefly recall the definitions of these Stokes-Dirac structures and port-Hamiltonian extensions for distributed parameter systems in the 1D case, with a spatial domain $\Omega = [0, L]$.

2.1. Hamiltonian formulation for systems of conservation laws

We shall define the conserved quantities as *1-forms* on the interval $\Omega = [0, L]$, whose space will be denoted $\Lambda^1(\Omega)$. Once a coordinate x (i.e. a measure dx) has been chosen on the interval Ω, the *1-form* $\alpha \in \Lambda^1(\Omega)$ may be written, using this coordinate, $\alpha = \alpha(x)\,dx$ where $\alpha(.)$ denotes a smooth function. The state space of a system of two conservation laws is the product space $\Lambda^1(\Omega) \times \Lambda^1(\Omega)$. The space of *0-forms*, that is smooth functions on the interval Ω, is denoted by $\Lambda^0(\Omega)$.

The symbol $\wedge$ will denote the exterior product of *k-forms* and d the exterior derivative.[2] We shall make use the Hodge star $\star$ operator associated with the measure dx of the real interval Ω. In the coordinate x, the Hodge star product of the *1-form* $\alpha(x)\,dx$ is simply the *0-form*: $\alpha(x)$.

Between *0-form* $\Lambda^0(\Omega) \ni \beta$ and *1-form* $\Lambda^1(\Omega) \ni \alpha$, one may define a bilinear form

$$\langle \beta | \alpha \rangle := \int_\Omega \beta \wedge \alpha \quad (\in \mathbb{R}) \tag{2.1}$$

which is simply expressed in coordinates as $\langle \beta | \alpha \rangle := \int_\Omega \beta(x)\,\alpha(x)\,dx$. The bilinear form (2.1), also referred in this paper as the natural *power-pairing*, is *non-degenerate* in the sense that if $\langle \beta | \alpha \rangle = 0$ for all α (respectively for all β), then $\beta = 0$ (respectively $\alpha = 0$). For real-valued functions $\gamma_i \in \Lambda^0(\partial\Omega)$, $i = 1, 2$ associated the spatial domain boundary $\partial\Omega = \{0,\ L\}$, we define the non-degenerated bilinear form:

$$\langle \gamma_1,\ \gamma_2 \rangle_\partial = \int_{\partial\Omega} \gamma_1 \wedge \gamma_2 = \gamma_1(L)\,\gamma_2(L) - \gamma_1(0)\,\gamma_2(0)$$

Consider an energy density *1-form* $\mathcal{H} : \Lambda^1(\Omega) \times \Omega \to \Lambda^1(\Omega)$ and denote by $H := \int_\Omega \mathcal{H} \in \mathbb{R}$ the associated Hamiltonian function. Then for any *1-form* $\omega \in \Lambda^1(\Omega)$ and any variation $\Delta\omega \in \Lambda^1(\Omega)$ with compact support strictly included in Ω and any $\kappa \in \mathbb{R}$, it may be proven that [29]:

$$H(\omega + \kappa\Delta\omega) = \int_\Omega \mathcal{H}(\omega + \kappa\Delta\omega) = \int_\Omega \mathcal{H}(\omega) + \kappa \int_\Omega \left[\frac{\delta H}{\delta \omega} \wedge \Delta\omega\right] + \mathrm{O}\left(\kappa^2\right)$$

for a uniquely defined *0-form* which will be denoted $\frac{\delta H}{\delta \omega} \in \Lambda^0(\Omega)$ and which is called the *variational derivative* of H with respect to $\alpha \in \Lambda^1(\Omega)$. It should be noticed that when $\mathcal{H}$ only depends on ω (and not

[1] Such pairs of conjugated variables are, for instance, the entropy density flow and the temperature in the thermal domain, the momentum density and the velocity in the kinetic domain, the pressure and the volumetric flow in the hydraulic domain, etc.

[2] Actually in the case of a 1D domain these operations become quite trivial. The wedge product of *0-forms*, i.e. functions, is simply their product and the wedge product of a *0-form* with a *1-form* is again simply the usual product of the *1-form* by the *0-form*. The only non-trivial exterior derivation acts on *0-forms* and is written with the coordinate x: $\mathrm{d}\beta(x) = \frac{\partial \beta}{\partial x}(x)\,dx$.