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Paul Kotyczka. Finite Volume Structure-Preserving Discretization of 1D Distributed-Parameter Port-Hamiltonian Systems. 2nd IFAC Workshop on Control of Systems Governed by Partial Differential Equations (CPDE 2016), IFAC, Jun 2016, Bertinoro, Italy. pp.300-305. hal-01350805

HAL Id: hal-01350805

<https://hal.science/hal-01350805>

Submitted on 1 Aug 2016

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Finite Volume Structure-Preserving Discretization of 1D Distributed-Parameter Port-Hamiltonian Systems

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Abstract: A family of finite-dimensional approximate models is proposed which preserves the port-Hamiltonian structure of a class of open systems of conservation laws. The approach is based on conservative generalized leapfrog schemes with given consistency orders in terms of their stencil. The finite volume perspective fits naturally to the formulation of the conservation laws on staggered grids. Some observations on current structure-preserving discretization methods are discussed and related to the proposed approach. A frequently used benchmark example highlights some of the method's properties and differences to existing structure-preserving schemes.

Keywords: Port-Hamiltonian systems, systems of conservation laws, distributed-parameter systems, semi-discretization, finite volume methods.

1. INTRODUCTION

The port-Hamiltonian (PH) representation of open systems of conservation laws [van der Schaft and Maschke 2002] captures their physical (interconnection) structure and in particular includes the expression of boundary port variables to describe the energy exchange with the environment. The latter is a prerequisite for boundary control, where the PH structure again is favorable in terms of well-posedness and the application of energy-based methods, see e.g. Ramirez et al. [2014]. A discretization of the underlying partial differential equations is necessary for simulation and, even more if nonlinear systems are considered, for manageable controller design. Different approaches for spatial semi-discretization which preserve the PH structure and in particular the power balance have been reported.

The core idea of structure-preserving semi-discretization methods for PH systems is to account for the different geometric nature of the power variables (efforts and flows) in the numerical approximation of their spatial distributions. Existing works are based on a (mixed) finite element (FE) perspective, using simple approximation forms on every segment [Golo et al. 2004] or higher order polynomials to approximate the distributed power variables at collocation points [Moulla et al. 2012]. A partial permutation of the canonical roles of energy and co-energy variables allows formulating an alternative structure-preserving discretization scheme [Farle et al. 2013].

For systems of conservation laws, there exists a multitude of finite volume (FV) / finite difference (FD) discretization schemes in space (semi-discretization) or in space and time (full-discretization) with different characteristic properties to simulate various systems and application cases. Find an overview of FD and FV methods for example in LeVeque [1992], LeVeque [2002], Eymard et al. [2000]. Among these methods, *conservative* schemes such as the *generalized leapfrog* methods [Iserles 1986] do not introduce numerical dissipation.

The purpose of this paper is to show that the semi-discrete versions of generalized leapfrog schemes are a very natural basis to formulate structure-preserving discretization methods for open PH systems of conservation laws. Thereby, naturally, special attention is paid to the definition of boundary port variables.

The paper is organized as follows. In Section 2, preliminaries on FV methods on staggered grids, semi-discrete leapfrog schemes and the PH representation of systems of two conservation laws in 1D are presented. Besides the distributed-parameter point of view, a discrete system representation on staggered grids, which serves as basis for the FV schemes in Section 4, is introduced. In Section 3, some observations on structure-preserving discretization of PH systems with current methods are summarized. Section 4 presents as a main result the class of FV semi-discretization methods for open PH systems. In Section 5, the illustrative example from Golo et al. [2004] is used for a first discussion and comparison of the presented approach. Section 6 concludes the paper with open questions and an outlook to further work.

* The author is on leave from Technical University of Munich at LAGEP with an Individual Fellowship of the European Commission's Marie Skłodowska-Curie Actions, Call H2020-MSCA-IF-2014_ST, Proposal No. 655204, EasyEBC – Easy-to-Implement Energy-Based Control Design for Systems of Conservation Laws.

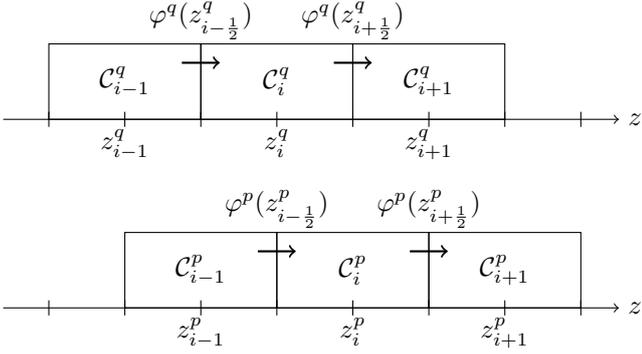


Fig. 1. Cells on both grids; fluxes at the cell boundaries.

2. PRELIMINARIES

2.1 Systems of two conservation laws

The dynamics of a (time-invariant) system of two conservation laws on a one-dimensional spatial domain can be represented in integral form by the equations¹

$$\frac{d}{dt} \int_{C_i^q} q(z, t) dz = \varphi^q(q, p, z_{i-1/2}^q, t) - \varphi^q(q, p, z_{i+1/2}^q, t) \quad (1)$$

$$\frac{d}{dt} \int_{C_i^p} p(z, t) dz = \varphi^p(q, p, z_{i-1/2}^p, t) - \varphi^p(q, p, z_{i+1/2}^p, t). \quad (2)$$

$q(z, t)$, $p(z, t)$ are the conserved quantities, $\mathcal{Z} = [z_L, z_R]$ the spatial domain, C_i^q , C_i^p are cells on the grid for the q and the p variable, respectively. φ^q , φ^p denote flux functions which are evaluated at the cell boundaries. z_i^q , z_i^p are the spatial coordinates of the cell centers. As depicted in Fig. 1, we consider *shifted* or *staggered* grids. This point of view, which is instrumental for achieving a certain consistency order with *generalized leapfrog* numerical schemes [Iserles 1986] can be found already in Yee et al. [1966] for the numerical simulation of Maxwell's equations. In differential form, (1), (2) correspond to

$$\frac{d}{dt} \begin{bmatrix} q(z, t) \\ p(z, t) \end{bmatrix} = - \frac{\partial}{\partial z} \begin{bmatrix} \varphi^q(q, p, z, t) \\ \varphi^p(q, p, z, t) \end{bmatrix} \quad (3)$$

with initial conditions $q(z, 0)$, $p(z, 0)$ and the corresponding boundary conditions on φ^q , φ^p at $z = z_L$, $z = z_R$.

Example. For the linear wave equation in first order representation we have $\varphi^q = p$, $\varphi^p = q$, and hence

$$\frac{d}{dt} \int_{C_i^q} q(z, t) dz = p(z_{i-1/2}^q, t) - p(z_{i+1/2}^q, t) \quad (4)$$

$$\frac{d}{dt} \int_{C_i^p} p(z, t) dz = q(z_{i-1/2}^p, t) - q(z_{i+1/2}^p, t). \quad (5)$$

2.2 Finite volume numerical schemes

A finite volume numerical scheme for this class of systems has the general structure²

$$\frac{d}{dt} Q_i = \phi_{i-1/2}^q - \phi_{i+1/2}^q \quad (6)$$

$$\frac{d}{dt} P_i = \phi_{i-1/2}^p - \phi_{i+1/2}^p. \quad (7)$$

¹ $\varphi^q(q, p, z_{i-1/2}^q, t)$ abbreviates $\varphi^q(q(z_{i-1/2}^q, t), p(z_{i-1/2}^q, t))$, etc.

² The time dependency is skipped for brevity.

Table 1. Coefficients for semi-discrete generalized leapfrog schemes with order $2r$

r	a_1	a_2	a_3
1	1		
2	$\frac{9}{8}$	$-\frac{1}{24}$	
3	$\frac{75}{64}$	$-\frac{25}{384}$	$\frac{3}{640}$

We denote

$$Q_i \approx \int_{C_i^q} q(z) dz, \quad P_i \approx \int_{C_i^p} p(z) dz \quad (8)$$

the numerical approximations of the integral conserved quantities on each cell and

$$\phi_{i\pm 1/2}^q \approx \varphi^q(q, p, z_{i\pm 1/2}^q), \quad \phi_{i\pm 1/2}^p \approx \varphi^p(q, p, z_{i\pm 1/2}^p) \quad (9)$$

the approximations of the boundary fluxes. These are computed from *numerical flux functions*, incorporating a finite number of approximate cell states Q_i , P_i , according to the *stencil* of the method. The simplest conservative finite volume method is the *leapfrog scheme* see e.g. Rezzolla [2011].

Example. The semi-discrete version (only in space) of the leapfrog scheme for the linear wave equation is

$$\begin{aligned} \dot{Q}_i &= \phi_{i-1/2}^q - \phi_{i+1/2}^q = P_{i-1} - P_i, \\ \dot{P}_i &= \phi_{i-1/2}^p - \phi_{i+1/2}^p = Q_i - Q_{i+1}. \end{aligned} \quad (10)$$

This numerical scheme has a consistency order of 2 in space and also in time, if an appropriate centered time integration step is considered [Iserles 1986], [Rezzolla 2011].

Higher consistency order of $2r$ with $r > 1$ can be obtained by *generalized leapfrog schemes* as presented in Iserles [1986] for the advection equation. $2r$ cells are taken into account to compute the net numerical fluxes into each cell.

Example. The generalized leapfrog scheme, adapted to the linear wave equation, reads

$$\begin{aligned} \dot{Q}_i &= \sum_{k=1}^r a_k (P_{i-k} - P_{i-1+k}) \\ \dot{P}_i &= \sum_{k=1}^r a_k (Q_{i+1-k} - Q_{i+k}). \end{aligned} \quad (11)$$

By computing the coefficients $1 \leq k \leq r$ according to³

$$a_k = (-1)^{r-k} \frac{(\mu - r + \frac{1}{2})2r}{(\mu - r + \frac{1}{2})(\mu + r - \frac{1}{2})(r-k)!(r-1+k)!}, \quad (12)$$

a consistency order of $2r$ in space is achieved. $\mu = \Delta t / \Delta z$ is the Courant number. With a centered scheme for time discretization, the correct μ has to be replaced. For the semi-discrete case with $\mu = 0$, the coefficients as in Table 5 of Fornberg and Ghrist [1999] are obtained.

2.3 Port-Hamiltonian systems of two conservation laws

In port-Hamiltonian form, the boundary fluxes are identified with point-wise evaluations of the *effort variables* on the dual grid. The latter are the variational derivatives

$$e^q(q, p, z) = \delta_q H(q, p), \quad e^p(q, p, z) = \delta_p H(q, p) \quad (13)$$

³ This is the semi-discrete version of the corresponding formula in Lemma 2 of Iserles [1986].

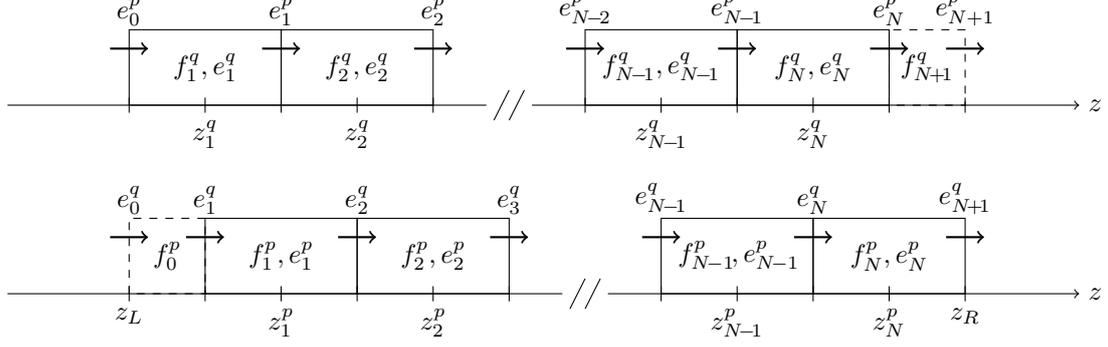


Fig. 2. Discrete representation of a system of two conservation laws with staggered control volumes (intervals). The boundary fluxes $e_0^p = e^p(z_L)$ and $e_{N+1}^q = e^q(z_R)$ are considered inputs, $e_0^q = e^q(z_L)$ and $-e_{N+1}^p = -e^p(z_R)$ collocated outputs. For the numerical schemes, the dashed control volumes are neglected, and $e_0^q \approx e_1^q$, $e_N^p \approx e_{N+1}^p$ is assumed.

of the total stored energy or Hamiltonian

$$H(q, p) = \int_0^L \mathcal{H}(q(z), p(z), z) dz. \quad (14)$$

with \mathcal{H} the Hamiltonian density. The PH dynamics in integral form is then given by⁴,

$$\frac{d}{dt} \int_{C_i^q} q(z, t) dz = e^p(q, p, z_{i-1}^p, t) - e^p(q, p, z_i^p, t) \quad (15)$$

$$\frac{d}{dt} \int_{C_i^p} p(z, t) dz = e^q(q, p, z_i^q, t) - e^q(q, p, z_{i+1}^q, t), \quad (16)$$

or, in differential form,

$$\frac{d}{dt} \begin{bmatrix} q(z, t) \\ p(z, t) \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \frac{\partial}{\partial z} \begin{bmatrix} e^q(z, t) \\ e^p(z, t) \end{bmatrix} \quad (17)$$

with appropriate initial and boundary conditions.

Example. The linear wave equation from the above examples is recovered when $\mathcal{H}(q, p) = \frac{q^2}{2} + \frac{p^2}{2}$.

A salient property of the PH representation is that, from the structure of the equations, using integration by parts (or Stokes theorem in more than one spatial dimension), the following power balance equation⁵ is obtained:

$$\dot{H} = \int_{z_L}^{z_R} e^q(z) \dot{q}(z) + e^p(z) \dot{p}(z) dz = - [e^q(z) e^p(z)]_{z_L}^{z_R}. \quad (18)$$

Stokes-Dirac structure. In a more formal way, see van der Schaft and Maschke [2002] for details, the power balance equation can be expressed as the *non degenerate bilinear form*, associated to the *Stokes-Dirac structure* on the space $\mathcal{F} \times \mathcal{E}$ defined by

$$\mathcal{F} = \Omega^1(\mathcal{Z}) \times \Omega^1(\mathcal{Z}) \times \Omega^0(\partial\mathcal{Z}) \ni (f^q, f^p, \mathbf{f}^b) \quad (19)$$

$$\mathcal{E} = \Omega^0(\mathcal{Z}) \times \Omega^0(\mathcal{Z}) \times \Omega^0(\partial\mathcal{Z}) \ni (e^q, e^p, \mathbf{e}^b) \quad (20)$$

with the one-forms (*flow variables* in $\Omega^1(\mathcal{Z})$)

$$f^q = \dot{q}(z) dz, \quad f^p = \dot{p}(z) dz, \quad (21)$$

the zero-forms (*effort variables* in $\Omega^0(\mathcal{Z})$) as defined above and the boundary variables (in $\Omega^0(\partial\mathcal{Z})$), defined e. g. as

$$\mathbf{e}^b = \begin{bmatrix} e^p(z_L) \\ e^q(z_R) \end{bmatrix}, \quad -\mathbf{f}^b = \begin{bmatrix} e^q(z_L) \\ -e^p(z_R) \end{bmatrix}. \quad (22)$$

⁴ Note that we have replaced $z_{i-1/2}^q = z_{i-1}^p$, $z_{i-1/2}^p = z_i^q$, etc.

⁵ Using the definition of the variational derivative and taking \dot{q} and \dot{p} as variations

The above-mentioned bilinear form to express the balance equation is then

$$\langle (e^q, e^p, \mathbf{e}^b) | (f^q, f^p, \mathbf{f}^b) \rangle = \int_{\mathcal{Z}} [e^q \wedge f^q + e^p \wedge f^p] + \langle \mathbf{e}^b, \mathbf{f}^b \rangle \quad (23)$$

with \wedge the exterior product between two differential forms, $\langle \cdot, \cdot \rangle$ the standard inner product on Euclidean space. Power-preservation is expressed by

$$\langle (e^q, e^p, \mathbf{e}^b) | (f^q, f^p, \mathbf{f}^b) \rangle = 0. \quad (24)$$

Discrete representation. As a whole, the system of two conservation laws can be represented in integral form by

$$\frac{d}{dt} \int_{z_L}^{z_R} q(z) dz = e^p(z_L) - e^p(z_R) \quad (25)$$

$$\frac{d}{dt} \int_{z_L}^{z_R} p(z) dz = e^q(z_L) - e^q(z_R), \quad (26)$$

which gives *no information about the spatial distribution* of the energy variables (states) $q(z)$ and $p(z)$. Dividing the spatial domain into the intervals

$$C_i^q = \begin{cases} [z_L, z_1^p] & i = 1, \\ (z_{i-1}^p, z_i^p] & i = 2, \dots, N, \end{cases} \quad (27)$$

$$C_i^p = \begin{cases} [z_i^q, z_{i+1}^q] & i = 1, \dots, N-1, \\ [z_N^q, z_R] & i = N, \end{cases} \quad (28)$$

the conservation laws can be rewritten, $i = 1, \dots, N$,

$$\frac{d}{dt} \int_{C_i^q} q(z) dz = e^p(z_{i-1}^p) - e^p(z_i^p), \quad (29)$$

$$\frac{d}{dt} \int_{C_i^p} p(z) dz = e^q(z_i^q) - e^q(z_{i+1}^q), \quad (30)$$

with $z_0^p = z_L$, $z_{N+1}^q = z_R$. Define for $i = 1, \dots, N$

$$f_i^q := \frac{d}{dt} \int_{C_i^q} q(z) dz, \quad f_i^p := \frac{d}{dt} \int_{C_i^p} p(z) dz, \quad (31)$$

as flow variables and the point-wise values of the distributed efforts

$$e_i^q := e^q(z_i^q), \quad e_i^p := e^p(z_i^p) \quad (32)$$

as efforts and collect them in the vectors

$$\mathbf{f}^q = \begin{bmatrix} f_1^q \\ \vdots \\ f_N^q \end{bmatrix}, \quad \mathbf{f}^p = \begin{bmatrix} f_1^p \\ \vdots \\ f_N^p \end{bmatrix}, \quad \mathbf{e}^q = \begin{bmatrix} e_1^q \\ \vdots \\ e_N^q \end{bmatrix}, \quad \mathbf{e}^p = \begin{bmatrix} e_1^p \\ \vdots \\ e_N^p \end{bmatrix}. \quad (33)$$

6. CONCLUSIONS

The proposed family of semi-discrete FV schemes provides ODE (control) models for the considered class of distributed-parameter PH systems with a given accuracy inside the spatial domain. An advantage compared to higher order FE or collocation methods is that the energy approximation to compute the co-state variables remains simple. The “parasitic” feedthrough which is present in some current structure-preserving methods is avoided. To increase the accuracy at the boundaries, additional measures have to be taken. The extension to higher spatial dimensions is conceptually simple in the FV perspective and is a topic of ongoing work, as well as the full-discretization to obtain multi-symplectic schemes for PH systems.

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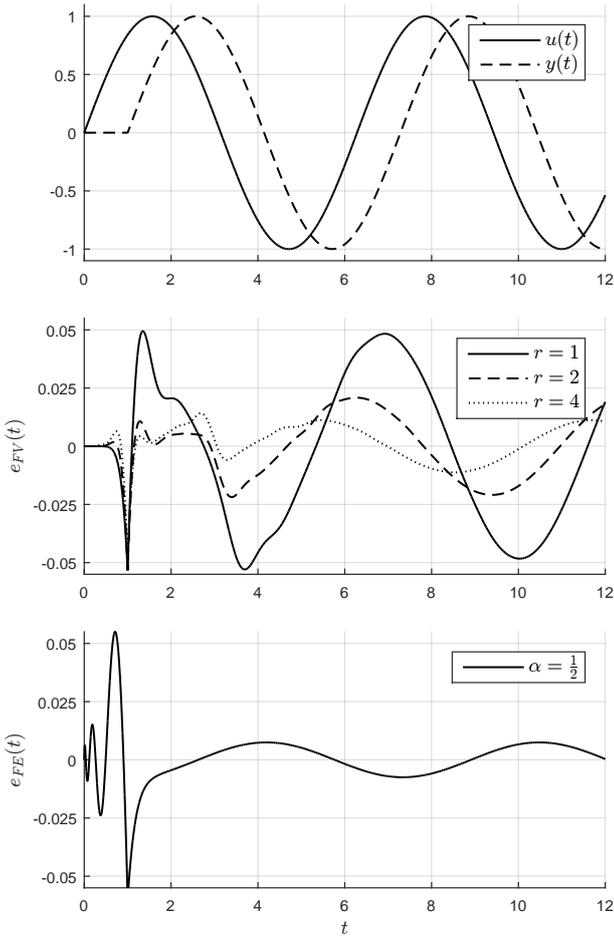


Fig. 3. Simulations of the non-constant transmission line. (a) Input and exact output voltage, (b) FV output error with three different stencils, (c) mixed FE simulation with $\alpha = 1/2$.

$\alpha = \frac{1}{2}$ (“Exp. 4”, spline approximation by Whitney forms, uniform grid) for comparison.

Each numerical experiment is based on a discretization with $N = 5$ segments, the lumped inductances, capacitances have been computed according to the expression indicated in Golo et al. [2004] for “Exp. 4”, replacing the cell centers on the accordingly shifted grids. The discretized models being linear, the simulations are conducted with MATLAB’s *lsim* with a step size of $h = 0.001$.

Avoiding a direct feedthrough in the discretized PH model, the FV scheme with staggered grids approximates the delay of the analytic solution in a non-oscillatory manner in the time interval $t \in [0, 1]$, in contrast to the mixed FE approximation. Increasing the order of the method by a wider stencil, the error $y_{FV,r}(t) - y(t)$ decreases for a fixed number of segments. The magnitude of the initial error around $t = 1$ remains practically unchanged. Increasing the number of segments⁷, the error norm of the numerical output decreases, yet not with order $(1/N)^{2r}$. This is due to the fact that no special measures to increase the accuracy at the boundaries, like appropriate *ghost cells*, have been implemented for the simulations.

⁷ which is not displayed for space limitation