Energy consistent schemes for port-Hamiltonian systems.

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Overview

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Port-Hamiltonian systems

Temporal discretisation

Numerical experiments (time discretisation)

Examples of port-Hamiltonian PDEs

Spatial discretisation

Energy based modelling

Port-Hamiltonian system/dissipative Hamiltonian systems:
Dynamics driven by energy functional $\mathscr{H} = \mathscr{H}(z)$ and split into energy conserving and energy dissipating mechanisms

$$C(z)\partial_t z = J(z)C(z)^T\mathscr{H}'(z) - R(z)C(z)^T\mathscr{H}'(z) + Bu \tag{PH}$$

with $J(z)$ skew symmetric, $R(z)$ symmetric positive definite, and B describes the effect of controls u.
Usually outputs are defined as $y = B^T\mathscr{H}'(z)$.

- Many important models such as gradient flows and compressible fluid dynamics can be written in such a form.
- The energy based viewpoint is very helpful for coupling different models.
- This form ensures fundamental properties such as passivity.

We will restrict ourselves to $C(z) = Id$.

Energy based modelling

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It is easy to check that solutions of (PH) satisfy a power balance

$$\partial_t \mathscr{H}(z) = \underbrace{-\mathscr{H}'(z)^T R(z) \mathscr{H}'(z)}_{\leq 0} + y^T u$$

Goal: Discretise (PH) so that a discrete power balance holds.

- We want energy decrease for $u = 0$
- We want energy conservation for $R = 0$, $u = 0$
- Also address the case where (PH) is a PDE.

Overview

Continuous Petrov-Galerkin for state independent J and R

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Final time $T > 0$, $m \in \mathbb{N}$. Consider time points $0 = t_0 < t_1 < ... < t_m = T$ and a partition of $[0, T]$ by subintervals

$$I_\tau := \{I_1, \dots, I_m\}, \text{ with } I_i := [t_{i-1}, t_i] \qquad \text{Set } \tau_i := t_i - t_{i-1}.$$

Let $\mathbb{P}_k(I_i; \mathbb{R}^n)$ denote polynomials of degree at most k mapping I_i to $\mathbb{R}^n$. We define spaces of piecewise polynomial functions

$$\mathbb{V}_k(I_\tau) := \{z \in L^\infty(I; \mathbb{R}^n) : z|_{I_i} \in \mathbb{P}_k(I_i; \mathbb{R}^n) \text{ for all } i\}, \quad \text{and}$$
$$\mathbb{V}_k^c(I_\tau) := \mathbb{V}_k(I_\tau; \mathbb{R}^n) \cap C(I; \mathbb{R}^n).$$

Petrov-Galerkin discretisation:
Seek $z_\tau \in \mathbb{V}_k^c(I_\tau)$ such that

$$\int_0^T \phi_\tau^T \partial_t z_\tau \, dt = \int_0^T \phi_\tau^T J \mathscr{H}'(z_\tau) - \phi_\tau^T R \mathscr{H}'(z_\tau) + \phi_\tau^T B u \, dt \quad \forall \phi_\tau \in \mathbb{V}_{k-1}(I_\tau)$$

For lowest order ($k = 1$) this is the Crank-Nicolson method

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Petrov-Galerkin discretisation can be localized:
Seek $z_\tau \in \mathbb{V}_k^c(I_\tau)$ such that

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Energy consistency for state independent J, R

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Let Π be L^2-orthogonal projection $\Pi : L^2(0, T; \mathbb{R}^n) \to \mathbb{V}_{k-1}(I_\tau)$ then we can use $\phi_\tau = \Pi(\mathscr{H}'(z_\tau))$ as test function: (use $u = 0$ for simplicity)

$$\int_{I_i} \Pi(\mathscr{H}'(z_\tau))^T \partial_t z_\tau \, dt = \int_{I_i} \Pi(\mathscr{H}'(z_\tau))^T J \mathscr{H}'(z_\tau) \; - \Pi(\mathscr{H}'(z_\tau))^T R \mathscr{H}'(z_\tau) \, dt$$

This implies

$$\int_{I_i} \mathscr{H}'(z_\tau)^T \partial_t z_\tau \, dt = \int_{I_i} \Pi(\mathscr{H}'(z_\tau))^T J \Pi(\mathscr{H}'(z_\tau)) - \Pi(\mathscr{H}'(z_\tau))^T \Pi(R\mathscr{H}'(z_\tau)) \, dt$$
$$= - \int_{I_i} \Pi(\mathscr{H}'(z_\tau))^T \Pi(R\mathscr{H}'(z_\tau)) \, dt \leq 0$$

Thus, $\mathscr{H}(z_\tau(t_i)) = \mathscr{H}(z_\tau(t_{i-1})) - \int_{I_i} \Pi(\mathscr{H}'(z_\tau))^T R \Pi(\mathscr{H}'(z_\tau))$.
Petrov-Galerkin schemes easily achieve the goal for J, R constant.

Modifying Petrov Galerkin I

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The proof shown above only works if J, R are independent of z, since, in general,

$$\int_{I_i} \Pi(\mathscr{H}'(z_\tau))^T J \Pi(\mathscr{H}'(z_\tau))\, dt \neq \int_{I_i} \Pi(\mathscr{H}'(z_\tau))^T J \mathscr{H}'(z_\tau)\, dt$$

First suggestion for a modified Petrov-Galerkin scheme: Seek $z_\tau \in \mathbb{V}_k^c(I_\tau)$ such that

$$\int_{I_i} \phi_\tau^T \partial_t z_\tau \, dt = \int_{I_i} \phi_\tau^T J(z_\tau)\Pi(\mathscr{H}'(z_\tau)) - \phi_\tau^T R(z_\tau)\Pi(\mathscr{H}'(z_\tau)) + \phi_\tau^T B u \, dt \quad \forall \phi_\tau \in \mathbb{P}_{k-1}(I_i;\mathbb{R}^n)$$

An analogous computation as above shows

$$\mathscr{H}(z_\tau(t_i)) = \mathscr{H}(z_\tau(t_{i-1})) - \int_{I_i} \Pi(\mathscr{H}'(z_\tau))^T R(z_\tau)\Pi(\mathscr{H}'(z_\tau)),$$

we get the desired energy consistency.

- Method is easy to implement: $(2k \cdot n) \times (2k \cdot n)$ system of equations in each time step.
- In practice we need a quadrature formula to compute the projection
- Introducing the projection is equivalent to introducing an auxiliary variable.

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An analogous computation as above shows

$$\mathcal{H}(z_\tau(t_i)) = \mathcal{H}(z_\tau(t_{i-1})) - \int_{I_i} \Pi(\mathcal{H}'(z_\tau))^T R(z_\tau)\Pi(\mathcal{H}'(z_\tau)),$$

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(Some) existing methods

- *Discrete gradient methods*: Gonzalez '96, McLachlan, Quispel & Robidoux '99 are exactly energy-preserving for Hamiltonian systems and, classically, of second order. High-order generalizations e.g.Eidnes '22, Schulze '23
- *Averaged vector field collocation methods* aka *energy-preserving collocation methods*: Hairer '10, Cohen & Hairer '11, Hairer & Lubich '14, Cellendoni & Hoiseth '17; exactly energy-preserving for Hamiltonian systems, energy-dissipating for gradient systems.
- Continuous Petrov-Galerkin methods using auxiliary variables: Morandin '24
- Continuous Petrov Galerkin methods preserving several invariants using multiple auxiliary variables: Andrews & Farrell '24

Rewriting the framework

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The equation

$$\partial_t z = \operatorname{sign}(z)\sqrt{|z|} = \frac{z}{\sqrt{z}}$$

fits into the above framework with $\mathscr{H}(z) = \frac{1}{2}z^2$ and $R(z) = \frac{1}{\sqrt{z}}$.
Here, the above discretisation creates a term of the form

$$\frac{\Pi(z_\tau)}{\sqrt{z_\tau}}$$

which is problematic: The denominator might be zero at certain points where the enumerator is not.

When we focus on cases where $\mathscr{H}$ is strictly convex, i.e. $\mathscr{H}'$ is invertible, then we can define $\tilde{J}$ such that $\tilde{J}(\mathscr{H}'(z)) = J(z)$ and absorb everything:

$$j(\eta, \phi) := \phi^T \tilde{J}(\eta)\eta, \quad r(\eta, \phi) := \phi^T \tilde{R}(\eta)\eta$$

Rewriting the framework II

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It seems more natural to consider problems of the form

$$\int_0^T \phi^T \partial_t z \, dt = \int_0^T j(\mathscr{H}'(z), \phi) - r(\mathscr{H}'(z), \phi) - \phi^T Bu \, dt \tag{PHnl}$$

for a suitable set of test functions ϕ.
Then, 'natural' numerical schemes read:
Seek $z_\tau \in \mathbb{V}_k^c(I_\tau)$ such that

$$\int_{I_i} \phi_\tau^T \partial_t z_\tau \, dt = \int_{I_i} j(\Pi(\mathscr{H}'(z_\tau)), \phi_\tau) - r(\Pi(\mathscr{H}'(z_\tau)), \phi_\tau) + \phi_\tau^T Bu \, dt \quad \forall \phi_\tau \in \mathbb{P}_{k-1}(I_i; \mathbb{R}^n)$$

or

$$\int_{I_i} \phi_\tau^T \partial_t z_\tau \, dt = Q_i \left[j(\Pi(\mathscr{H}'(z_\tau)), \phi_\tau) - r(\Pi(\mathscr{H}'(z_\tau)), \phi_\tau) + \phi_\tau^T Bu \right] \quad \forall \phi_\tau \in \mathbb{P}_{k-1}(I_i; \mathbb{R}^n)$$

for some quadrature Q_i.
We have energy conservation/dissipation as long as Q_i has non-negative weights.

Overview

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Example 1: the Toda lattice

We describe the motion of a chain of particles in 1D. Each particle is connected to its nearest neighbors with an exponential spring. Let the control exert a force on the first particle.
For N particles, $q \in \mathbb{R}^N$ denotes their displacement vector and $p \in \mathbb{R}^N$ their momentum. We set $z := (q, p)^T$ and have the form (PH) with

$$J = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix} \in \mathbb{R}^{2N\times 2N}, \quad R = \begin{pmatrix} 0 & 0 \\ 0 & \operatorname{diag}(\gamma_1, \dots, \gamma_N) \end{pmatrix} \in \mathbb{R}^{2N\times 2N}, \quad B = \begin{pmatrix} 0 \\ e_1 \end{pmatrix} \in \mathbb{R}^{2N\times 1}.$$

Here $I_N \in \mathbb{R}^{N\times N}$ is the identity matrix, $\gamma_i \geq 0$ are given damping parameters, and e_1 is the first unit vector.
The Hamiltonian of the system reads

$$\mathscr{H}(z) = \sum_{k=1}^{N} \frac{1}{2} p_k^2 + \sum_{k=1}^{N-1} \exp(q_k - q_{k+1}) + \exp(q_N - q_1) - N$$

Varying polynomial degrees k

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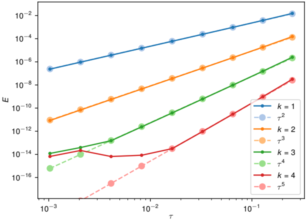
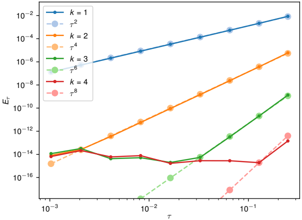
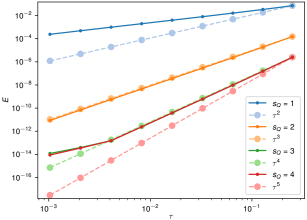
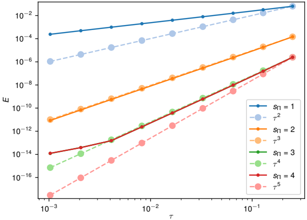




Left: Optimal decay rates in L^∞ for different polynomial degrees k
Right: Nodal super convergence (order $2k$) for different polynomial degrees k

Varying numbers of quadrature points





Left: Varying the number of (Gauss) quadrature nodes s_Q in Q_i

Right: Varying the number of (Gauss) quadrature nodes s_Π for computing the projection

$\Rightarrow$ Taking $s_Q = k = s_\Pi$ seems optimal.

Example 2: Spinning rigid body

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A rigid body spinning around its center of mass in the absence of gravity can be modeled by (PH) with $z = (p_1, p_2, p_3)^T$ the vector of angular momenta of the body and

$$\tilde{J}(z) = \begin{pmatrix} 0 & -p_3 & p_2 \\ p_3 & 0 & -p_1 \\ -p_2 & p_1 & 0 \end{pmatrix}, \; R = 0, \quad \text{and} \quad \tilde{B} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix},$$

where $\tilde{B}$ is the axis around which torque is applied, and $u \in \mathbb{R}$ is a given control. The Hamiltonian

$$\mathscr{H}(z) = \frac{1}{2} \sum_{i=1}^{3} I_i z_i^2$$

is quadratic with $I_1, I_2, I_3 > 0$ the principal moments of inertia.

Simulation rigid spinning body

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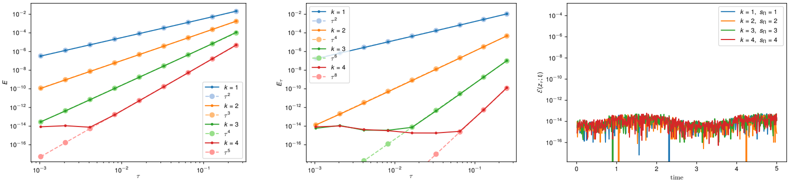

Left: Decay of L^∞ error: order $(k + 1) \Rightarrow$ optimal.
Middle: Decay of nodal error: order $(2k) \Rightarrow$ nodal super convergence.
Right: Energy conservation up to 10^{-14} nearly machine precision.

Overview

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Examples of port-Hamiltonian PDEs

Spatial discretisation

Example 1: Quasilinear wave equation

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$$\partial_t \rho + \operatorname{div}(v) = 0,$$
$$\partial_t v + \operatorname{div}(p(\rho)) = -F(v) + \nu \Delta v,$$

with boundary conditions

$$(p(\rho) I - \nu \nabla v) n = g \text{ on } (0, T) \times \partial\Omega$$

where n is the unit outer normal. Set $z = (\rho, v)^T$ and

$$\mathcal{H}(z) := \int_\Omega P(\rho) + \frac{1}{2} |v|^2 \, \mathrm{d}x \qquad \text{for } P(\rho) := \int_0^\rho p(r) \, \mathrm{d}r.$$

Then, $\mathscr{H}'(z) = (p(\rho), v)$ and for any $\phi = (\xi, w)^T$ we have

$$\int_\Omega \partial_t z \cdot \phi \, \mathrm{d}x = \underbrace{\int_\Omega p(\rho) \operatorname{div}(w) - \operatorname{div}(v)\, \xi \, \mathrm{d}x}_{=:j(\mathscr{H}'(z),\phi)=j((p(\rho),v),\phi)} - \underbrace{\int_\Omega F(v) \cdot w + \nu \nabla v : \nabla w \, \mathrm{d}x}_{=:r(\mathscr{H}'(z),\phi)} - \underbrace{\int_{\partial\Omega} g \cdot w \, \mathrm{d}\sigma}_{\text{boundary 'control'}},$$

Expl 2: Doubly nonlinear parabolic equations

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We consider strictly monotone functions $\alpha : \mathbb{R} \to \mathbb{R}$ and $\beta : \mathbb{R}^n \to \mathbb{R}^n$ and the PDE

$$\partial_t z - \operatorname{div}\left(\beta\left(\nabla(\alpha^{-1}(z))\right)\right) = 0.$$

with boundary conditions:

$$\beta(\nabla\alpha^{-1}(z)) \cdot n = 0 \text{ on } (0, T) \times \partial\Omega$$

This has the form (PHnl) with $j = 0$,

$$\mathscr{H} \text{ such that } \mathscr{H}'(z) = \alpha^{-1}(z), \quad \text{and} \quad r(\chi, \phi) = \int_\Omega \beta(\nabla\chi) \cdot \nabla\phi.$$

Several popular models have this form:

- porous medium equation
- p-Laplace equation
- 'ISO3' model describing friction dominated flow in gas pipelines:

$$z = \rho, \quad \eta'(\rho) = \rho p'(\rho), \quad \text{and} \quad \beta(q) = \frac{q}{\sqrt{|q|}}$$

Overview

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Spatial discretisation I

In ODEs: $j : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$, $r : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$
In PDEs: $j : X \times X \to \mathbb{R}$, $r : X \times X \to \mathbb{R}$ where X is some (infinite dimensional) Banach space:

- Wave equation: $X = L^2(\Omega) \times H^1(\Omega)$
- Doubly nonlinear parabolic model: $X = W^{1,p}(\Omega)$ for some suitable $p > 1$.

j, r are linear in their second arguments and satisfy

$$j(\chi, \chi) = 0, \;\; r(\chi, \chi) \geq 0$$

Method of lines:

- Discretise the problem in space such that we obtain a finite dimensional ODE of the form (PHnl).
- Apply time discretisation as described above.

Spatial discretisation I

Let $X_h \subset X \subset L^2(\Omega)$ finite dimensional, then a Galerkin spatial semi-discretisation would be ($u = 0$ for brevity) to seek $z_h \in C^1([0,T], X_h)$ such that

$$\int_\Omega \phi_h^T \partial_t z_h \, \mathrm{d}x = j(\mathscr{H}'(z_h), \phi_h) - r(\mathscr{H}'(z_h), \phi_h) \quad \forall \phi_h \in X_h$$

This does not satisfy an energy balance! However, when $\Pi_h : X \to X_h$ denotes L^2-orthogonal projection, we may consider

$$\int_\Omega \phi_h^T \partial_t z_h \, \mathrm{d}x = j(\Pi_h(\mathscr{H}'(z_h)), \phi_h) - r(\Pi_h(\mathscr{H}'(z_h)), \phi_h) \quad \forall \phi_h \in X_h$$

which satisfies an energy balance:

$$\frac{d}{dt}\mathscr{H}(z_h) = -r(\Pi_h(\mathscr{H}'(z_h), \Pi_h(\mathscr{H}'(z_h))$$

Spatial discretisation II

The discretisation

$$\int_\Omega \phi_h^T \partial_t z_h \,\mathrm{d}\,x = j(\Pi_h(\mathscr{H}'(z_h)), \phi_h) - r(\Pi_h(\mathscr{H}'(z_h)), \phi_h) \quad \forall \phi_h \in X_h \tag{$*$}$$

is of the form (PHnl) with

$$j_h(\chi, \phi_h) := j(\Pi_h(\chi), \phi_h), \quad r_h(\chi, \phi_h) := r(\Pi_h(\chi), \phi_h)$$

- Introducing the projection is equivalent to introducing and auxiliary variable in the sense that $(*)$ is equivalent to

$$\int_\Omega \phi_h^T \partial_t z_h \,\mathrm{d}\,x = j(\chi_h, \phi_h) - r(\chi_h, \phi_h) \quad \forall \phi \in X_h$$
$$\int_\Omega \psi_h^T \chi_h \,\mathrm{d}\,x = \int_\Omega \psi_h^T \mathscr{H}'(z_h) \,\mathrm{d}\,x \quad \forall \psi \in X_h$$

- Standard Galerkin form, but size doubled.

Convergence in τ for quasilinear wave equation

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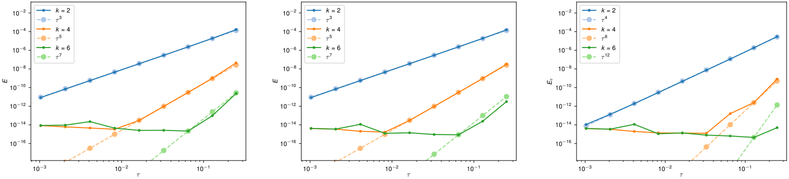

Left: $\nu = 0$ convergence in $L^\infty(0, T; L^2(\Omega))$ for $\tau \to 0$.
Middle: $\nu = 1$ convergence in $L^\infty(0, T; L^2(\Omega))$ for $\tau \to 0$.
Right: $\nu = 1$ nodal super convergence in $\ell^\infty(\{t_i\}; L^2(\Omega))$ for $\tau \to 0$.

Convergence in τ for quasilinear wave equation

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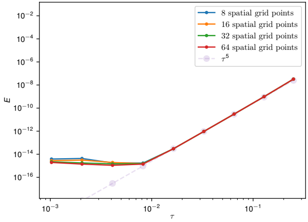

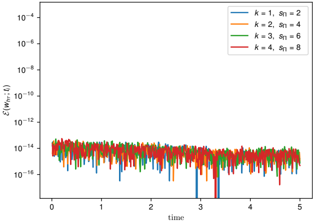

Left: $\nu = 1$ convergence in $L^\infty(0, T; L^2(\Omega))$ for $\tau \to 0$ is uniform in h

Right: $\nu = 1$ error in energy balance

Summary and Outlook

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- Systematic way to construct *structure preserving* space and time discretisations of port- Hamiltonian systems
- Similar methods have been used case by case for space discretisation in many special cases before
- Order is optimal (relative to polynomial degree) and arbitrary (can be increased by increasing polynomial degree)
- Discretisation is of Galerkin type ("simple") but doubles systems size

- Systematic investigation of $h \to 0$ limit
- A priori and a posteriori error estimates
- Generalizing the class of systems: $C(z)\partial_t z$ instead of $\partial_t z$

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Thank you for your attention!