Structure-preserving Reduced Complexity Modelling

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Outline

Reduced Complexity Modelling

Motivation: Parametric PDEs and Solution Manifolds

- multi-query contexts (optimisation, inverse problems, control, ...) require the repeated solution of parametric partial differential equations
- denote the parameter space by $\mathbb{P} \subset \mathbb{R}^p$ and the solution (Hilbert) space by V
- parametrised PDE problem for $u \in V$ and $\mu \in \mathbb{P}$

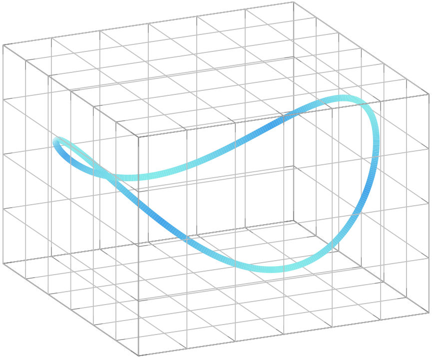
$$F(u(\mu); \mu) = 0$$

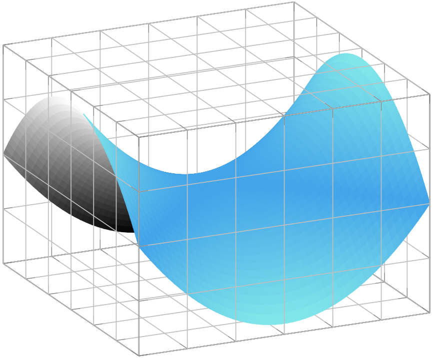
- numerical algorithms seek approximate solutions $u_h \approx u$ in finite-dimensional spaces $V_h \approx V$; typically u_h is represented by a degree-of-freedom vector $\hat{u} \in \mathbb{R}^{N_h} \simeq V_h$ where $N_h = \dim V_h$
- with traditional numerical methods, the space V_h is typically not adapted to the problem and therefore needs to be rather large, resulting in high computational costs
- the actual solution manifold $\mathcal{M}$ is typically a much smaller space

$$\mathcal{M} = \{u(\mu) \in V : F(u(\mu); \mu) = 0,\ \mu \in \mathbb{P}\} \subset V_h$$

Motivation: Parametric PDEs and Solution Manifolds

- the solution manifold $\mathcal{M} = \{u(\mu) \in V : F(u(\mu); \mu) = 0,\ \mu \in \mathbb{P}\} \subset V$ is typically a very small space





- goal: construct an approximation of the solution manifold $\mathcal{M}_h$ and the embedding map $\mathcal{M}_h \hookrightarrow V_h$

Data-driven Model Order Reduction

- Strategy: Learn a low-dimensional representation of a system that captures relevant physical properties
- from a dataset M of solutions $\hat{u}(\mu)$ for different values of the parameter μ construct
    - a mapping $\mathcal{P}$ from V_h to the low-dimensional space V_r (reduction)
    - a mapping $\mathcal{R}$ from the low-dimensional space V_r to V_h (reconstruction)
    - a reduced representation $\tilde{u} \in V_r$ such that $\mathcal{R}\tilde{u}(\mu) \approx \hat{u}(\mu)$ and $\dim(V_r) \ll \dim(V_h)$
    - a reduced system of equations $\tilde{F}(\tilde{u}(\mu); \mu) = 0$
- the mappings $\mathcal{P}$ and $\mathcal{R}$ are chosen such that they minimise the reconstruction error:

$$\min_{\mathcal{P},\mathcal{R}} \frac{1}{2} ||\mathsf{M} - \mathcal{R} \circ \mathcal{P}(\mathsf{M})||^2$$

- in order to obtain accurate reduced oder models, important properties of the high order model, such as symplecticity or conservation of invariants, need to be accounted for in the construction of $\mathcal{P}$, $\mathcal{R}$ and $\tilde{F}$

Application: Particle Discretisation of the Vlasov–Poisson System

- Vlasov–Poisson system for the dynamics of a charged particle distribution f

$$\frac{\partial f}{\partial t}(t,x,v) + v \cdot \frac{\partial f}{\partial x}(t,x,v) - \nabla\phi(x) \cdot \frac{\partial f}{\partial v}(t,x,v) = 0, \qquad -\Delta\phi(t,x) = \int f(t,x,v)\,dv$$

- particle discretisation of f, Galerkin discretisation of ϕ

$$f_h(t,x,v) = \sum_{a=1}^{N_p} w_a\,\delta(x - x_a(t))\,\delta(v - v_a(t)), \qquad \phi_h(t,x) = \sum_{i=1}^{N_\phi} \phi_i(t)\,\psi_i(x)$$

- semi-discrete equations of motion

$$\begin{pmatrix} \dot{x}_a(t) \\ \dot{v}_a(t) \end{pmatrix} = \begin{pmatrix} v_a(t) \\ -\nabla_x \phi_h(t, x_a) \end{pmatrix}, \quad \mathsf{K}_{ij}\phi_j(t) = \sum_{a=1}^{N_p} w_a\,\psi_i(x_a(t)), \quad \mathsf{K}_{ij} = \int \nabla\psi_i(x) \cdot \nabla\psi_j(x)\,dx$$

- state vectors of all particles in position space, velocity space, and phase space

$$\hat{X} = (x_1,\,\dots,\,x_{N_p})^T, \qquad \hat{V} = (v_1,\,\dots,\,v_{N_p})^T, \qquad \hat{u} = (x_1,\,\dots,\,x_{N_p},\,v_1,\,\dots,\,v_{N_p})^T$$

Hamiltonian Dynamics

Hamiltonian Systems

- general, finite dimensional Hamiltonian or Poisson system

$$\dot{z} = \mathcal{P}(z)\,\nabla H(z), \qquad z \in \mathcal{M} = \mathbb{R}^m$$

with $\mathcal{P}(z)$ an anti-symmetric matrix, possibly degenerate, satisfying

$$\sum_{l=1}^{m} \left(\frac{\partial \mathcal{P}^{ij}(z)}{\partial z^l} \mathcal{P}^{lk}(z) + \frac{\partial \mathcal{P}^{jk}(z)}{\partial z^l} \mathcal{P}^{li}(z) + \frac{\partial \mathcal{P}^{ki}(z)}{\partial z^l} \mathcal{P}^{lj}(z) \right) = 0$$

- canonical symplectic: constant Poisson structure $\mathcal{P} = \mathbb{J}_{2d}^{-1}$

$$\mathbb{J}_{2d} = \begin{pmatrix} \mathbb{0}_d & -\mathbb{1}_d \\ \mathbb{1}_d & \mathbb{0}_d \end{pmatrix}$$

- natural splitting: $z = (q, p)$

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \qquad \frac{dp}{dt} = -\frac{\partial H}{\partial q}, \qquad i = 1, ..., d$$

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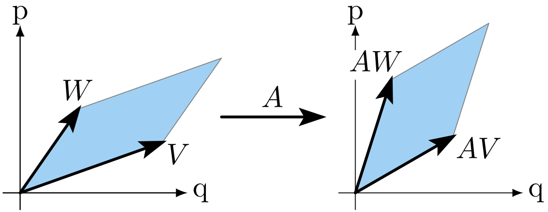
Symplectic Maps

- the flow ϕ_H of a Hamiltonian system is a symplectic map of the phasespace into itself

$$(p^1, q^1) = \phi_H(t_1, t_0)(p^0, q^0)$$

- a linear map $A : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is called symplectic if $A^T \Omega A = \Omega$ with Ω a symplectic matrix
- a nonlinear map $\phi : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is called symplectic if $(\mathrm{D}\phi)^T \Omega (\mathrm{D}\phi) = \Omega$
- consequences: preservation of phasespace area as well as higher Poincaré integral invariants
- symplecticity dramatically restricts the number of dynamically accessible states compared to non-symplectic systems
- symplecticity is a characteristic property of Hamiltonian (and Lagrangian) systems



Reduced Basis Methods

Reduced Basis Methods

- find a small set of reduced basis functions $\{\zeta_i\}_{i=1}^n$ and write reduced representation of solutions as

$$\tilde{u}(\mu) = \sum_{i=1}^{n} \tilde{u}_i(\mu)\,\zeta_i$$

→ How can we construct such a set of reduced basis vectors?

  - Proper orthogonal decomposition selects the eigenvectors of the empirical correlation operator of solution snapshots for different values of the parameters μ obtained from a high fidelity integrator
  - Offline phase: limited number of simulations with high fidelity method and computation of reduced basis
  - Online phase: many (cheap) simulations with reduced basis

→ Other approaches:

  - Autoencoders, a special type of neural network architecture, are designed to map a high dimensional space to a low dimensional feature space (intrinsic manifold)
  - ...

Proper Orthogonal Decomposition

- collect snapshots $\{\hat{u}^{(j)} = \hat{u}(\mu_j)\}_{j=1}^{n_s} \subset V_h$ of solutions for $\mu_j \in \mathbb{P}$ and compose a snapshot matrix

$$\mathsf{S} = \left[\hat{u}^{(1)} \mid \ldots \mid \hat{u}^{(n_s)}\right] \in \mathbb{R}^{N_h \times n_s}$$

- singular value decomposition of the snapshot matrix $\mathsf{S} = \mathsf{V}\Sigma\mathsf{Z}^T$ yields orthonormal ζ_i as columns of V
- discrete solutions are approximated as linear combinations of the first n eigenvectors ζ_i

$$\tilde{u}(\mu) = \sum_{i=1}^{n} \tilde{u}_i(\mu)\,\zeta_i, \qquad \mathsf{V}^T = \begin{pmatrix} \zeta_{1,1} & \cdots & \zeta_{1,n} \\ \vdots & & \vdots \\ \zeta_{n,1} & \ldots & \zeta_{n,n} \end{pmatrix}, \qquad \zeta_i = \begin{pmatrix} \zeta_{i,1} \\ \vdots \\ \zeta_{i,n} \end{pmatrix}$$

- truncating $\mathsf{V} = \left[\zeta_1 \mid \ldots \mid \zeta_n\right]$ yields the reduced basis as well as the reconstruction and reduction operators $\mathcal{R} = \mathsf{V}$ and $\mathcal{P} = \mathsf{V}^T$ such that the reconstruction error satisfies

$$\sum_{i=1}^{n_s} \frac{1}{2}||u^{(i)} - \mathsf{V}\mathsf{V}^T u^{(i)}||^2 = \text{minimum among all } n\text{-dimensional orthogonal bases}$$

Galerkin Projection

- recall the discrete Vlasov–Poisson system (omitting time dependencies for clearity)

$$\begin{pmatrix} \dot{x}_a \\ \dot{v}_a \end{pmatrix} = \begin{pmatrix} v_a \\ -\nabla_{x_a} \Phi(\hat{X}) \end{pmatrix}, \qquad \Phi(\hat{X}) = \sum_{a=1}^{N_p} \phi_h(x_a), \qquad \mathsf{K}_{ij}\phi_j = \sum_{a=1}^{N_p} w_a \, \psi_i(x_a) = \Psi_i(\hat{X})$$

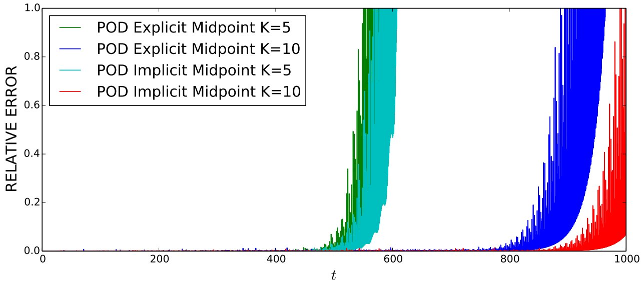
- replacing $\hat{u} = (\hat{X}, \hat{V})^T \in \mathbb{R}^{2N_p}$ with the reduced basis representation $\mathsf{V}\tilde{u} = (\mathsf{V}_x\tilde{X}, \mathsf{V}_v\tilde{V}) \in \mathbb{R}^{2n}$ yields a system of $2N_p$ equations for $2n$ degrees-of-freedom with $n \ll N_p$

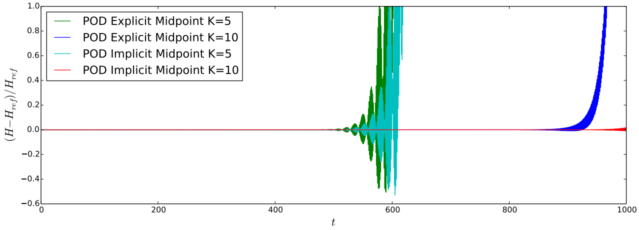
$$\begin{pmatrix} (\mathsf{V}_x\dot{\tilde{X}})_a \\ (\mathsf{V}_v\dot{\tilde{V}})_a \end{pmatrix} = \begin{pmatrix} (\mathsf{V}_v\tilde{V})_a \\ -\nabla_{x_a} \Phi_h(\mathsf{V}_x\tilde{X}) \end{pmatrix}, \qquad \mathsf{K}_{ij}\phi_j = \Psi_i(\mathsf{V}_x\tilde{X})$$

- Galerkin projection with V^T yields a (dense) system of $2n$ equations (note that $\mathsf{V}^T\mathsf{V} = \mathbb{I}$)

$$\begin{pmatrix} \dot{\tilde{X}} \\ \dot{\tilde{V}} \end{pmatrix} = \begin{pmatrix} \mathsf{V}_x^T\mathsf{V}_v\tilde{V} \\ -\mathsf{V}_v^T \nabla_{\hat{X}} \Phi_h(\mathsf{V}_x\tilde{X}) \end{pmatrix}, \qquad \mathsf{K}_{ij}\phi_j(t) = \Psi_i(\mathsf{V}_x\tilde{X})$$

Proper Orthogonal Decomposition





Proper Symplectic Decomposition

- Proper Symplectic Decomposition constraints the possible matrices to a subset of the symplectic lifts

$$\min_{\mathsf{V}} \frac{1}{2} \left|\left|\mathsf{S} - \mathsf{V}\mathsf{V}^T\mathsf{S}\right|\right|^2 \qquad \text{with} \qquad \mathsf{V} = \begin{pmatrix} \mathsf{A} & \mathbb{0} \\ \mathbb{0} & \mathsf{A} \end{pmatrix}, \qquad \mathsf{S} = \left[\mathsf{S}_q \,\middle|\, \mathsf{S}_p\right]$$

→ A consists of the first n columns of V for $\left[\mathsf{S}_q \,\middle|\, \mathsf{S}_p\right] = \mathsf{V}\Sigma\mathsf{Z}^T$

- Galerkin projection with the symplectic inverse $\mathsf{V}^+ = \mathbb{J}_{2n}\mathsf{V}^T\mathbb{J}_{2N}^T$ again yields a Hamiltonian system

$$\frac{d\tilde{X}}{dt} = \frac{\partial\tilde{H}}{\partial\tilde{V}}, \qquad \frac{d(\tilde{\mathsf{M}}\tilde{V})}{dt} = -\frac{\partial\tilde{H}}{\partial\tilde{X}}, \qquad \tilde{H}(\tilde{X},\tilde{V}) = \frac{1}{2}\tilde{V}^T\tilde{\mathsf{M}}\tilde{V} + \Phi(\mathsf{V}\tilde{X}), \qquad \tilde{\mathsf{M}} = \mathsf{V}^T\mathsf{M}\mathsf{V}$$

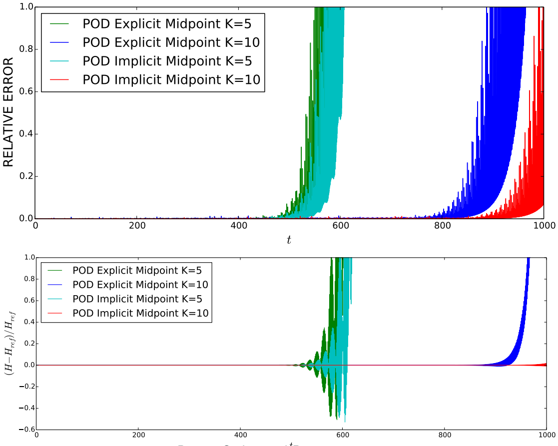
or equivalently

$$\dot{\hat{Z}} = \mathsf{V}^+\mathbb{J}_{2N}\nabla H(\mathsf{V}\hat{Z}) = \mathbb{J}_{2n}\mathsf{V}^T\mathbb{J}_{2N}^T\mathbb{J}_{2N}\nabla H(\mathsf{V}\hat{Z}) = \mathbb{J}_{2n}\mathsf{V}^T\nabla H(\mathsf{V}\hat{Z})$$

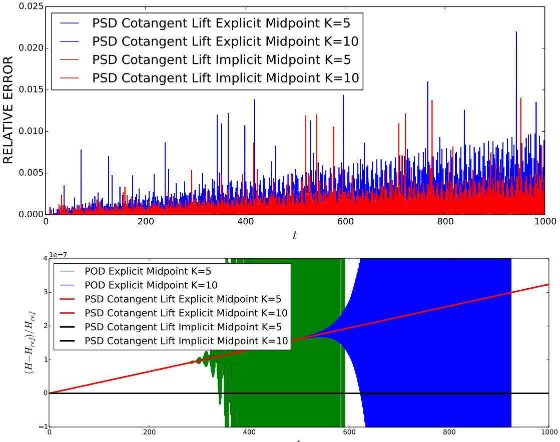
- applying a symplectic integrator on the low-dimensional PSD system yields a discrete symplectic flow

H. Peng, N. Song, Z. Kan. Data-driven model order reduction with proper symplectic decomposition for flexible multibody system. Nonlinear Dynamics 107.1, pp. 173–203, 2022.

POD vs. PSD



Proper Orthogonal Decomposition



Proper Symplectic Decomposition

Structure-preserving Hyper-reduction

- challenge: structure-preserving reduction of nonlinear operators (hyper-reduction)
- evaluation of the potential Φ is expensive due to the reconstruction of the high-order solution

$$\frac{d\tilde{X}}{dt} = \frac{\partial \tilde{H}}{\partial \tilde{V}} = \tilde{V}, \qquad \frac{d(\tilde{\mathsf{M}}\tilde{V})}{dt} = -\frac{\partial \tilde{H}}{\partial \tilde{X}} = \mathsf{V}^T \nabla \Phi(\mathsf{V}\tilde{X}), \qquad \tilde{H}(\tilde{X}, \tilde{V}) = \frac{1}{2}\tilde{V}^T \tilde{\mathsf{M}} \tilde{V} + \Phi(\mathsf{V}\tilde{X})$$

- standard hyper-reduction methods like Discrete Empirical Interpolation Method (DEIM) or Dynamic Mode Decomposition (DMD) do not account for symplectic structure of the vector field

$$\frac{d\tilde{X}}{dt} = \tilde{V}, \qquad \frac{d(\tilde{\mathsf{M}}\tilde{V})}{dt} = \mathsf{V}^T \Pi_{\mathsf{DEIM}} \nabla \Phi(\mathsf{I}_{\mathsf{DEIM}} \mathsf{V}\tilde{X})$$

- solution: do not perform hyper-reduction of the vector field but on the Hamiltonian

$$\tilde{H}_{\mathsf{DEIM}}(\tilde{X}, \tilde{V}) = \frac{1}{2}\tilde{V}^T \tilde{\mathsf{M}} \tilde{V} + \Phi_{\mathsf{DEIM}}(\tilde{X}), \qquad \Phi_{\mathsf{DEIM}}(\tilde{X}) = \Phi(\Pi_{\mathsf{DEIM}}^T \mathsf{V}\tilde{X})$$

  - approximate $\Phi(\mathsf{V}\tilde{X})$ by a Hamiltonian Neural Network $\Phi_{\mathsf{HNN}}(\tilde{X})$
  - replace standard symplectic integrator on reduced vector field with a SympNet

Summary

Structure-preserving Reduced Complexity Modelling

- **Main Message:** Preserving structure in model reduction is important!

- **Limitations of Reduced Basis Methods:**
  - reduction of nonlinear operators
  - advection-dominated problems

  → **Talk by Benedikt Brantner:** Symplectic Autoencoders

  → **Poster by Tobias Blickhan:** Transport Maps

Structure-preserving Reduced Complexity Modelling

Solution Space	Time Integration
• high fidelity • reduced basis • symplectic reduced basis • autoencoder • symplectic autoencoder	• symplectic or variational integrator • HNNs / LNNs for nonlinear operators • HNNs / LNNs for collective dynamics • SympNets / symplectic LSTMs

Implementation in Julia: `https://github.com/JuliaGNI`, `https://github.com/JuliaRCM`