Structure-preserving Reduced Complexity Modelling

Reduced Basis Methods and Scientific Machine Learning

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Outline

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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 $\hat{u} \in \mathbb{R}^{N_h} \simeq V_h$
- 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

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

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 to the low-dimensional space $\mathcal{P}$ (reduction)
  - a mapping from the low-dimensional space $\mathcal{R}$ (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

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

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

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

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 snapshots of solutions for different values of the parameters μ obtained from a high fidelity integrator

→ 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

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

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

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

- truncating $\mathsf{V} = \left[\zeta_1 \,|\, \dots \,|\, \zeta_n\right]$ 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)

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

- 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 system of $2n$ equations (note that $\mathsf{V}^T\mathsf{V} = \mathbb{I}$)

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

Hamiltonian Dynamics

Hamiltonian Dynamics

- the dynamics of (canonical) Hamiltonian systems is determined by the Hamiltonian function H by

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \qquad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}$$

  or equivalently

$$\dot{z} = \mathbb{J}_{2N_p} \nabla H(z), \qquad z = (q,p)^T, \qquad \mathbb{J}_{2N} = \begin{pmatrix} \mathbb{0}_{N_p} & \mathbb{1}_{N_p} \\ -\mathbb{1}_{N_p} & \mathbb{0}_{N_p} \end{pmatrix}$$

- the particle discretisation of the Vlasov–Poisson system fits this form with $q = x$ and $p = mv$

$$\frac{dx^a}{dt} = \frac{\partial H}{\partial v_a}, \qquad \frac{d(m_a v_a)}{dt} = -\frac{\partial H}{\partial x_a}, \qquad H(\hat{X}, \hat{V}) = \frac{1}{2}\hat{V}^T \mathsf{M} \hat{V} + \Phi(\hat{X})$$

- the flow of a Hamiltonian system
  - preserves the total energy of the system H
  - is a symplectic map of the phase space into itself

→ the Hamiltonian structure of the system should be preserved during model order reduction

Proper Symplectic Decomposition

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

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

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

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

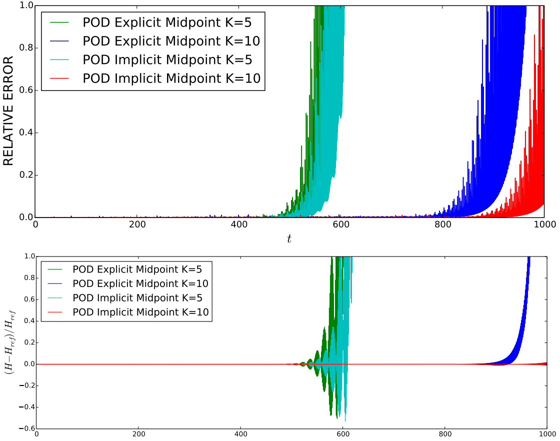
$$\frac{d\tilde{X}}{dt} = \frac{\partial \tilde{H}}{\partial \tilde{V}}, \qquad \frac{d(\tilde{\mathsf{M}}\tilde{V})}{dt} = -\frac{\partial \tilde{H}}{\partial \tilde{X}}, \qquad \tilde{H}(\tilde{X}, \tilde{V}) = \frac{1}{2}\tilde{V}^T\tilde{\mathsf{M}}\tilde{V} + \Phi(\mathsf{V}\tilde{X}), \qquad \tilde{\mathsf{M}}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

or equivalently

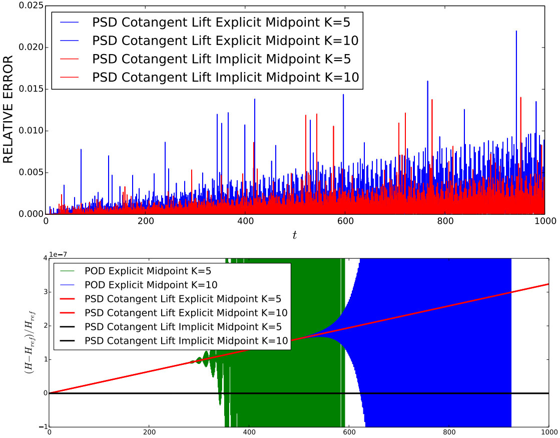
$$\dot{\hat{Z}} = \mathsf{V}^+\mathbb{J}_{2N}\nabla H(\mathsf{V}\hat{Z}) = \mathbb{J}_{2n}\mathsf{V}^T\mathbb{J}_{2N}^T\mathbb{J}_{2N}\nabla H(\mathsf{V}\hat{Z}) = \mathbb{J}_{2n}\mathsf{V}^T\nabla H(\mathsf{V}\hat{Z})$$

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

Proper Orthogonal Decomposition vs. Proper Symplectic Decomposition



Proper Orthogonal Decomposition



Proper Symplectic Decomposition

Structure-preserving 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 DEIM or DMD that approximate nonlinearities in the vector field do not account for symplectic structure

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

- crucial: do not perform hyper-reduction of the vector field but on the Hamiltonian
  - approximate $\Phi(\mathsf{V}\tilde{X})$ by a neural network $\tilde{\Phi}(\tilde{X})$, that provides a differentiable map $\tilde{\Phi} : \mathbb{R}^n \to \mathbb{R}$ (replaces solution of the Poisson equation and evaluation of the potential on all particle positions)
  - ...

Outlook: Symplectic Autoencoders

- autoencoders are a special type of neural network architectures, designed to map a high dimensional space (the data) to a low dimensional feature space (intrinsic manifold)
- they consist of an encoder $\Psi^{\mathrm{enc}}_{\theta_1} : \mathbb{R}^N \to \mathbb{R}^n$ and a decoder $\Psi^{\mathrm{dec}}_{\theta_2} : \mathbb{R}^n \to \mathbb{R}^N$, both of which are neural networks, parametrized by θ_1 and θ_2 respectively
- both are trained simultaneously on a data set M to minimize the **reconstruction error**

$$L(\theta) := \frac{1}{2} ||M - \Psi^{\mathrm{dec}}_{\theta_2} \circ \Psi^{\mathrm{enc}}_{\theta_1}(M)||^2$$

- training is usually done via some version of gradient descent

$$\theta \leftarrow \theta - \eta \nabla_\theta L(\theta) \qquad \text{with } \eta \text{ the learning rate}$$

- autoencoders can be used for model reduction in a similar fashion as reduced basis methods

→ see B. Brantner's talk on symplectic autoencoders on Friday (*Contributed Talks Session 14, N-130*)

Poisson Brackets

Hamiltonian Dynamics and Poisson Brackets

- let $u(t, x) = (u^1, u^2, \ldots, u^m)^T$ be the field variables of some system of partial differential equations, defined over the space Ω with coordinates x
- for Hamiltonian systems the evolution of any functional $\mathcal{F}$ of the field variables u is given by

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F}, \mathcal{H}\} \qquad \text{with} \qquad \{\mathcal{F}, \mathcal{G}\} = \int\limits_{\Omega} \frac{\delta \mathcal{F}}{\delta u^i} \, \mathcal{J}^{ij}(u) \, \frac{\delta \mathcal{G}}{\delta u^j} \, \mathrm{d}x$$

- $\mathcal{F}$, $\mathcal{G}$ and $\mathcal{H}$ are functionals of u and $\delta \mathcal{F} / \delta u^i$ is the functional derivative
- specifically, $\mathcal{H}$ is the Hamiltonian functional, usually the total energy of the system
- the Poisson bracket $\{\cdot, \cdot\}$ is an bilinear, anti-symmetric operation that satisfies Leibniz' rule and the Jacobi identity,

$$\{\{\mathcal{F}, \mathcal{G}\}, \mathcal{H}\} + \{\{\mathcal{G}, \mathcal{H}\}, \mathcal{F}\} + \{\{\mathcal{H}, \mathcal{F}\}, \mathcal{G}\} = 0,$$

for arbitrary functionals $\mathcal{F}, \mathcal{G}, \mathcal{H}$ of u

Hamiltonian Dynamics and Poisson Brackets

- for Hamiltonian systems, the evolution of any functional $\mathcal{F}$ is given by

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F}, \mathcal{H}\} \qquad \text{with} \qquad \{\mathcal{F}, \mathcal{G}\} = \int\limits_{\Omega} \frac{\delta \mathcal{F}}{\delta u^i} \, \mathcal{J}^{ij}(u) \, \frac{\delta \mathcal{G}}{\delta u^j} \, \mathrm{d}z$$

- Hamiltonian systems preserve energy due to anti-symmetry of the Poisson bracket

$$\frac{d\mathcal{H}}{dt} = \{\mathcal{H}, \mathcal{H}\} = -\{\mathcal{H}, \mathcal{H}\} = 0$$

- if the Hamiltonian is constant along the flow of some functional $\mathcal{P}$, i.e., $\{\mathcal{H}, \mathcal{P}\} = 0$, then $\mathcal{P}$ is a momentum map that is preserved by the flow of $\mathcal{H}$ as

$$\frac{d\mathcal{P}}{dt} = \{\mathcal{P}, \mathcal{H}\} = -\{\mathcal{H}, \mathcal{P}\} = 0$$

- if $\mathcal{J}(u)$ has a non-empty nullspace, there exist so-called Casimir invariants, that is functionals $\mathcal{C}$ for which $\{\mathcal{F}, \mathcal{C}\} = 0$ for all functionals $\mathcal{F}$, i.e.,

$$\mathcal{J}^{ij}(u) \, \frac{\delta \mathcal{C}}{\delta u^j} = 0$$

Burgers Equation

- Burgers Equation

$$\partial_t u + 3u\,\partial_x u = 0$$

- conservation law form

$$\partial_t u + \frac{3}{2}\partial_x(u^2) = 0$$

- Poisson Bracket

$$\{\mathcal{F}, \mathcal{G}\}[u] = -\int u \left(\frac{\delta \mathcal{F}}{\delta u} \frac{\partial}{\partial x} \frac{\delta \mathcal{G}}{\delta u} - \frac{\delta \mathcal{G}}{\delta u} \frac{\partial}{\partial x} \frac{\delta \mathcal{F}}{\delta u} \right) \mathrm{d}x$$

$$\mathcal{H} = \frac{1}{2} \int |u|^2 \; \mathrm{d}x$$

Discretisation of Poisson Brackets: Discrete Functionals

- choose a finite dimensional function space

$$V_h = \big\{ u_h = u_h(x) \,:\, u_h|_{\Omega_i} \in \mathbb{P}^r(\Omega_i) \big\}$$

- when evaluated on the discrete field variable u_h, any linear functional $\mathcal{F}[u]$ turns into a function $F(\hat{u})$ of the degrees of freedom $\hat{u}$

$$F(\hat{u}) = \mathcal{F}[u_h]$$

- example: Hamiltonian of the Burgers equation

$$H(\hat{u}) = \mathcal{H}[u_h] = \frac{1}{2} \int\limits_{\Omega} u_h^2 \, dx = \frac{1}{2} \, \hat{u}^T M \, \hat{u}, \qquad M_{ij} = \int\limits_{\Omega} \phi_i(x) \, \phi_j(x) \, dx$$

- the functional derivates of $\mathcal{F}$, when restricted to discrete solutions u_h, can be approximated by partial derivatives of F with respect to the degrees of freedom $\hat{u}$

Discretisation of Poisson Brackets: Discrete Functional Derivatives

- let the functional derivative be defined as the L^2-representative of the Fréchet derivative

$$\langle D\mathcal{F}[u]\,,\,v\rangle_{L^2} = \int_\Omega \frac{\delta \mathcal{F}}{\delta u}\cdot v\,dx$$

- let $\{\phi_i\}_{i=1}^N$ denote a basis in V_h and $\{\psi_i\}_{i=1}^N$ the dual basis in V_h^*, such that $\langle \psi_i\,,\,\varphi_j\rangle_{L^2} = \delta_{ij}$
- the functional derivative can be expressed in the dual basis as

$$\frac{\delta \mathcal{F}}{\delta u}[u_h](x) = \sum_i \frac{\partial F}{\partial u_i}\,\psi_i(x) = \sum_{i,j} \frac{\partial F}{\partial u_i}\mathsf{M}_{ij}^{-1}\,\varphi_j(x)$$

- we can write the discrete Poisson bracket as

$$\{F,G\}_d = \sum_{i,l,m} c_{im}^l u_l\,\frac{\partial F}{\partial u_i}\,\frac{\partial G}{\partial u_m},$$

$$c_{im}^l = -\sum_{j,n} \mathsf{M}_{ij}^{-1}\,\mathsf{M}_{mn}^{-1}\int_{\Omega_k}\varphi_l(x)\left(\varphi_n(x)\frac{\partial}{\partial x}\varphi_j(x) - \varphi_j(x)\frac{\partial}{\partial x}\varphi_n(x)\right)\mathrm{d}x$$

Discretisation of Poisson Brackets

- dynamical equations of motion

$$\dot{u}_i = \{u_i, H\}_d, \qquad H(\hat{u}) = \frac{1}{2} \sum_{i,j} u_i M_{ij} u_j, \qquad M_{ij} = \int_\Omega \phi_i(x)\, \phi_j(x)\, dx$$

  thus

$$\dot{u}_i = \sum_{j,l,m} c^l_{jm} u_l \frac{\partial u_i}{\partial u_j} \frac{\partial H}{\partial u_m} = \sum_{j,k,l,m} c^l_{jm} u_l\, \delta_{ij}\, M_{mk} u_k = \sum_{k,l,m} c^l_{im} u_l\, M_{mk} u_k$$

- the discretisation of Poisson brackets automatically leads to energy- and often other invariant-preserving methods

- open problem: Jacobi-identity-preserving truncation

→ good starting point for energy- and invariant-preserving reduced basis methods

Discretised Poisson Brackets and Reduced Bases

- reduced basis Poisson bracket: replace u_i with $\mathsf{V}^T_{ij}\tilde{u}_j$ and apply the chain rule

$$
\begin{aligned}
\{F, G\}_r &= \sum_{i,j,k,l,m,n} c^l_{im} \mathsf{V}^T_{ln} \tilde{u}_n \frac{\partial F}{\partial \tilde{u}_j} \frac{\partial \tilde{u}_j}{\partial u_i} \frac{\partial G}{\partial \tilde{u}_k} \frac{\partial \tilde{u}_k}{\partial u_m} \\
&= \sum_{i,j,k,l,m,n} c^l_{im} \mathsf{V}^T_{ln} \tilde{u}_n \frac{\partial F}{\partial \tilde{u}_j} \mathsf{V}_{ji} \frac{\partial G}{\partial \tilde{u}_k} \mathsf{V}_{km} \\
&= \sum_{i,j,k,l,m,n} \tilde{c}^n_{jk} \tilde{u}_n \frac{\partial F}{\partial \tilde{u}_j} \frac{\partial G}{\partial \tilde{u}_k} \\
\tilde{c}^l_{im} &= c^l_{jk} \mathsf{V}^T_{ln} \mathsf{V}^T_{ij} \mathsf{V}^T_{mk}
\end{aligned}
$$

- combining discretised Poisson brackets with reduced bases automatically leads to energy-preserving reduced basis methods and conservation of other invariants is easily checked
- caution: if the functional derivative of the Hamiltonian is not well represented in the reduced basis, this approach might lead to increased errors

→ see T. Blickhan's talk on Friday (*Contributed Talks Session 14, N-130*)

Summary and Outlook

Summary and Outlook

- Symplectic reduced basis methods show improved stability and reduced error growth over standard proper orthogonal decomposition
- Hamilton and Lagrangian formulations facilitate structure-preserving hyper-reduction
- Energy-preserving reduced basis methods can easily be constructed by combination of discretised Poisson brackets and reduced bases
- Symplectic Autoencoders: see B. Brantner's talk on Friday (*Contributed Talks Session 14, N-130*)
- Invariant-preserving reduced basis methods: see T. Blickhan's talk on Friday (*Contributed Talks Session 14, N-130*)

Appendix: Lagrangian Reduction of the Vlasov–Poisson System

Particle Model for Vlasov–Poisson

- charged particle equations with phase space coordinates $z = (x, v)$ in an electrostatic potential ϕ

$$\begin{pmatrix} \dot{x} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} v \\ -\nabla_x \phi(x) \end{pmatrix}$$

- Poisson equation

$$-\Delta \phi = \rho(x_1, \, ..., \, x_N)$$

- state vector of all particles in phase space

$$Z = (x_1, \, ..., \, x_N, \, v_1, \, ..., \, v_N)^T \in \mathbb{R}^{2N}$$

- phase space Lagrangian

$$L(Z, \dot{Z}, \phi) = \sum_{a=1}^{N} \Big(v_a^T M \dot{x}_a - \frac{1}{2} v_a^T M v_a - \phi(x_a) \Big) + \frac{1}{2} \int\limits_{\Omega} \left| \nabla \phi(x) \right|^2 dx$$

Model Order Reduction

- structure-preserving reduced basis $\tilde{Z} \in \mathbb{R}^n$ obtained e.g. via PSD, such that

$$\tilde{Z} = U^T Z \qquad \text{with reconstruction} \qquad Z = U\tilde{Z} \qquad \text{where} \qquad U^T U = \mathrm{Id}_n$$

- reduced equations of motion (still symplectic)

$$U\dot{\tilde{Z}} = \begin{pmatrix} U_v \tilde{Z} \\ -\nabla_x \phi(U_x \tilde{Z}) \end{pmatrix} \qquad \text{where} \qquad U = \begin{pmatrix} U_x \\ U_v \end{pmatrix} \qquad \text{so that} \qquad X = U_x \tilde{Z}, \quad V = U_v \tilde{Z}$$

- ϕ is obtained self-consistently from the particle distribution

$$\phi_j \int \nabla\varphi_i \cdot \nabla\varphi_j = \sum_{a=1}^{N} \varphi_i(x_a) \qquad \text{with} \qquad \phi(t,x) = \sum_{i=1}^{M} \phi_i(t)\, \varphi_i(x)$$

- two problems: in the evaluation of the gradient of ϕ in the force term, and in the projection of the particles onto the basis of ϕ, we need to reconstruct the particle positions from the reduced basis $\tilde{Z}$

Learning the Electrostatic Potential

- goal: obtain an expression of ϕ directly in terms of the reduced basis $\tilde{Z}$
- added benefit: structure-preserving reduction of nonlinearity (not possible with DEIM or DMD)
- training (offline) phase: solve the system of particles and alongside compute and store ϕ and construct the reduced basis from the training data
- for each step in each training simulation, construct a map

$$\tilde{Z} \mapsto \tilde{\Phi}(\tilde{Z}) = \Phi(U_{x,a}\tilde{Z}) = \sum_a \phi(U_{x,a}\tilde{Z}), \qquad \Phi(Z) = \sum_a \phi(x_a)$$

  (Φ holds the total electrostatic potential summed over all reconstructed particle positions)

- $\tilde{\Phi}$ is represented by a neural network, that constitutes a differentiable map $\tilde{Z} \mapsto \tilde{\Phi}$ from $\mathbb{R}^n$ to $\mathbb{R}$ (replaces solution of the Poisson equation and evaluation of the potential on all particle positions)

Reduced Basis Lagrangian

- phase space particle Lagrangian (Φ enters only as prescribed function)

$$L(Z, \dot{Z}; \Phi) = \sum_{a=1}^{N} \Big(v_a^T M \dot{x}_a - \tfrac{1}{2} v_a^T M v_a - \phi(x_a) \Big)$$

- reduced basis Lagrangian

$$L(\tilde{Z}, \dot{\tilde{Z}}; \tilde{\Phi}) = \sum_{a=1}^{N} \Big(\tilde{Z}^T U_{v,a}^T M U_{x,a} \dot{\tilde{Z}} - \tfrac{1}{2} \tilde{Z}^T U_{v,a}^T M U_{v,a} \tilde{Z} - \phi(U_{x,a} \tilde{Z}) \Big)$$

- neural network Lagrangian: the last term, $\phi(U_{x,a}\tilde{Z})$, is replaced with the neural network $\tilde{\Phi}(\tilde{Z})$

$$\tilde{L}(\tilde{Z}, \dot{\tilde{Z}}; \tilde{\Phi}) = \tilde{Z}^T \tilde{M}_{vx} \dot{\tilde{Z}} - \tfrac{1}{2} \tilde{Z}^T \tilde{M}_{vv} \tilde{Z} - \tilde{\Phi}(\tilde{Z})$$

with

$$\tilde{M}_{vx} = U_v^T (\mathbb{1} \otimes M)\, U_x, \qquad \tilde{M}_{vv} = U_v^T (\mathbb{1} \otimes M)\, U_v, \qquad \tilde{\Phi}(\tilde{Z}) = \sum_a \phi(U_{x,a} \tilde{Z})$$

- variations with respect to $\tilde{Z}$ yield Euler-Lagrange equations in the reduced basis

Collective Dynamics

- reduced basis $\tilde{Z} = U^T Z$ with reconstruction $Z = U\tilde{Z}$, such that $U^T U = \mathrm{Id}_n$ and

$$U = \begin{pmatrix} U_q \\ U_p \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} Q \\ P \end{pmatrix} = \begin{pmatrix} U_q \\ U_p \end{pmatrix} \tilde{Z} \qquad \text{or} \qquad U = \begin{pmatrix} U_q \\ U_v \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} Q \\ V \end{pmatrix} = \begin{pmatrix} U_q \\ U_v \end{pmatrix} \tilde{Z}$$

- no explicit treatment of the electrostatic potential Φ
- train HNN or LNN on the reduced basis

$$\mathcal{L}_{\mathsf{HNN}} = \left\| U_q \frac{\partial H_\theta}{\partial \tilde{P}} - \dot{Q} \right\|_2 + \left\| U_p \frac{\partial H_\theta}{\partial \tilde{Q}} + \dot{P} \right\|_2, \qquad (\tilde{Q}_0, \tilde{P}_0) \mapsto (\tilde{Q}_1, \tilde{P}_1)$$

$$\mathcal{L}_{\mathsf{LNN}} = \left\| U_v \left(\frac{\partial^2 L_\theta}{\partial \dot{\tilde{Q}}\, \partial \dot{\tilde{Q}}} \right)^{-1} \left(\frac{\partial L_\theta}{\partial \tilde{Q}} - \frac{\partial^2 L_\theta}{\partial \dot{\tilde{Q}}\, \partial \tilde{Q}} \tilde{V} \right) - \dot{V} \right\|_2 + \left\| U_q \dot{\tilde{Q}} - \dot{Q} \right\|_2, \qquad (\tilde{Q}_0, \tilde{V}_0) \mapsto (\tilde{Q}_1, \tilde{V}_1)$$

$$\mathcal{L}^{\mathsf{nc}}_{\mathsf{HNN}} = \left\| U \left(\tilde{\nabla} \vartheta_\theta - \tilde{\nabla} \vartheta_\theta^T \right)^{-1} \tilde{\nabla} H_\theta - \dot{Z} \right\|_2, \qquad (\tilde{Z}_0) \mapsto (\tilde{Z}_1)$$

$$\mathcal{L}^{\mathsf{nc}}_{\mathsf{LNN}} = \left\| U \left(\frac{\partial^2 L_\theta}{\partial \dot{\tilde{Z}}\, \partial \tilde{Z}} \right)^{-T} \frac{\partial L_\theta}{\partial \tilde{Z}} - \dot{Z} \right\|_2, \qquad (\tilde{Z}_0) \mapsto (\tilde{Z}_1)$$