SAND2023-07573C

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Canonical and Noncanonical Hamiltonian Model Reduction through Benchmark Examples

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Workshop on Data-Driven Modeling of Physical Systems, USC, 4/6/2023

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Hamiltonian Systems

- Archetype for conservative systems: $\dot{\mathbf{x}} = \{\mathbf{x}, H\} = \mathbf{L}\nabla H$.
  - Governed by scalar potential function *H* and SS matrix $\mathbf{L}$.
- $\mathbf{L}$ defines (potentially degenerate) Poisson bracket $\{F, G\} = \nabla F \cdot \mathbf{L}\nabla G$.
  - Satisfies Jacobi identity $\{F, \{G, H\}\} + \{G, \{H, F\}\} + \{H, \{F, G\}\} = 0$.
- Guarantees that flow is $\perp \nabla H$ and energy is conserved:

$$\dot{H}(\mathbf{x}) = \dot{\mathbf{x}} \cdot \nabla H = \mathbf{L}\nabla H \cdot \nabla H = -\mathbf{L}\nabla H \cdot \nabla H = 0 .$$

Examples of Hamiltonian systems

GIFs courtesy of Wikipedia under Creative Commons license

- Undamped simple harmonic oscillator: $m\ddot{x} = -kx$

$$H = \frac{1}{2m}\left(p^2 + q^2\right) \qquad \mathbf{L} = \mathbf{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

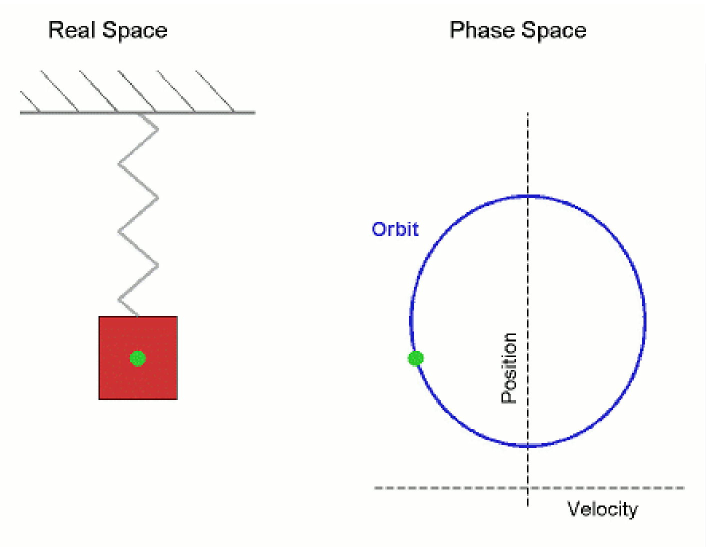
$$p = m\dot{x}, \quad q = m\sqrt{\frac{k}{m}}x$$

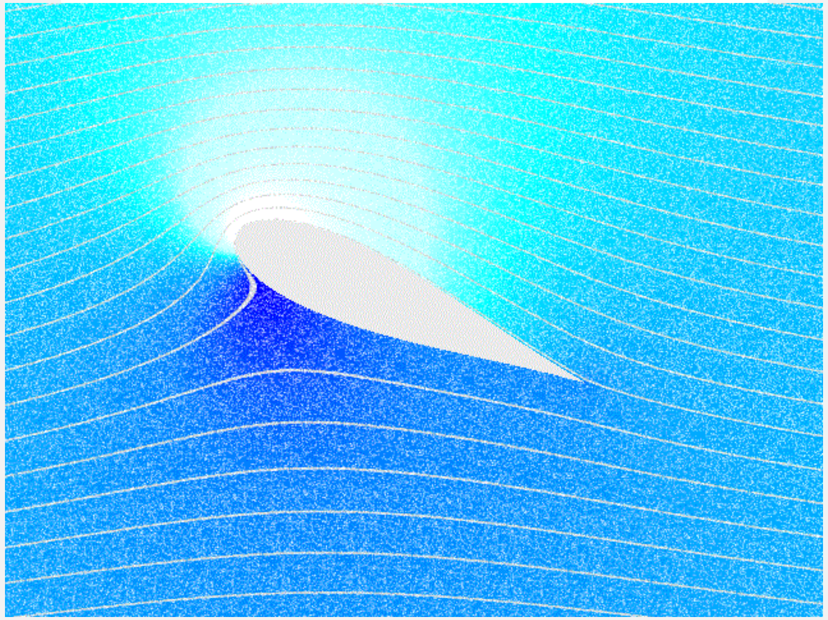
- Incompressible Euler: $\dot{\boldsymbol{\omega}} = \boldsymbol{\omega} \cdot \nabla \mathbf{u} - \mathbf{u} \cdot \nabla \boldsymbol{\omega}$

$$H = \frac{1}{2}\int |\mathbf{u}|^2 \, dx. \quad L(\boldsymbol{\omega}) = (\boldsymbol{\omega} \cdot \nabla - \nabla \boldsymbol{\omega})\, \nabla \times$$

  - Warning! Vorticity is the Hamiltonian variable!

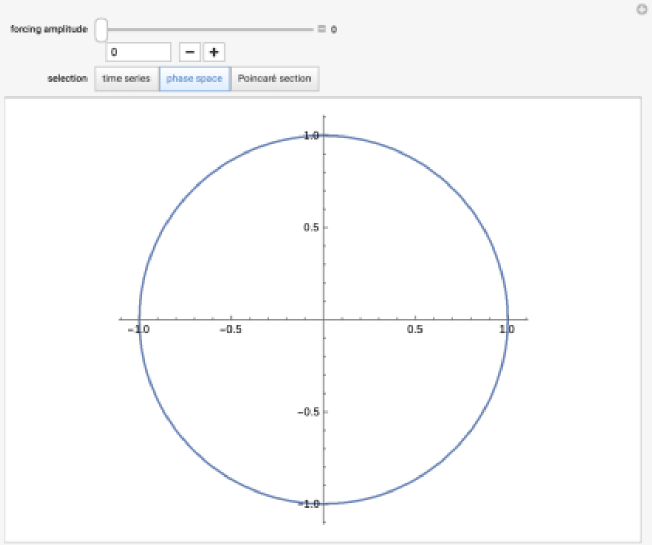
$$\boldsymbol{\omega} = \nabla \times \mathbf{u}$$

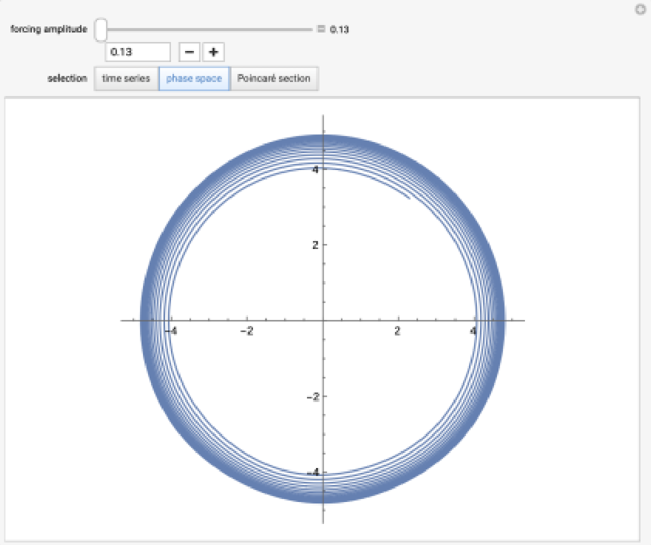




Why do we like Hamiltonian systems?

- Dynamics governed by *one* function.
  - Generally chaotic but controlled. Phase space volume doesn't change.
  - KAM theorem: "small" perturbations of integrable system yield "small" changes in periodicity.
- Connection with geodesics on Riemannian manifolds.
  - Optimal transport





https://demonstrations.wolfram.com/KAMToriReforming/

Proper Orthogonal Decomposition

- Suppose $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{f}(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^N$ large.
- Do PCA on solution snapshots $\boldsymbol{X} = \boldsymbol{x}(t_j, \boldsymbol{\mu}_j),\ 1 \le j \le N_t$.
  - Yields $\mathbf{X} \approx \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^\intercal$, Galerkin projection $\tilde{\mathbf{x}} = \mathbf{U}\hat{\mathbf{x}}$.
- Orthogonality of POD basis $\mathbf{U}$ implies, for $\hat{\mathbf{x}} \in \mathbb{R}^n,\ \hat{f} = f \circ \tilde{\mathbf{x}}$,

$$\dot{\hat{\mathbf{x}}} = \mathbf{U}^\intercal \mathbf{A}\mathbf{U}\hat{\mathbf{x}} + \mathbf{U}^\intercal \mathbf{f}\left(\mathbf{U}\hat{\mathbf{x}}\right) := \hat{\mathbf{A}}\hat{\mathbf{x}} + \hat{\mathbf{f}}\left(\hat{\mathbf{x}}\right)$$

- ODE of size *N* converted to ODE of size *n*.

1D wave equation

$$h(s) = \begin{cases} 1 - \frac{3}{2}s^2 + \frac{3}{4}s^3 & 0 \le s \le 1, \\ \frac{1}{4}(2-s)^3 & 1 \le s \le 2, \\ 0 & s > 2. \end{cases}$$

$s(x) = 10|x - \frac{1}{2}|$ Initial condition

- Want to solve $\frac{\partial^2 \varphi}{\partial t^2} = c^2 \frac{\partial^2 \varphi}{\partial x^2},$
- Recast as $q = \varphi$ and $p = \varphi_t$ $\quad \mathcal{H}(q,p) = \int_0^\ell \left[\frac{1}{2}p^2 + \frac{1}{2}c^2 q_x^2 \right] \mathrm{d}x,$
- Discretization yields $H_d(\mathbf{y}) = \sum_1^n \left[\frac{1}{2}p_i^2 + \frac{c^2(q_{i+1}-q_i)^2}{4\Delta x^2} + \frac{c^2(q_i - q_{i-1})^2}{4\Delta x^2} \right]$
  - Assume periodic BCs
- FOM system is $\dot{\mathbf{y}} = \mathbf{J}_{2n} \nabla_{\mathbf{y}} H_d(\mathbf{y}) = \begin{bmatrix} \mathbf{0} & \mathbf{I}_n \\ -\mathbf{I}_n & \mathbf{0} \end{bmatrix} \begin{bmatrix} -c^2 \mathbf{D}_{fd} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_n \end{bmatrix} \mathbf{y} = \begin{bmatrix} \mathbf{0} & \mathbf{I}_n \\ c^2 \mathbf{D}_{fd} & \mathbf{0} \end{bmatrix} \mathbf{y}.$

Is standard POD good enough?

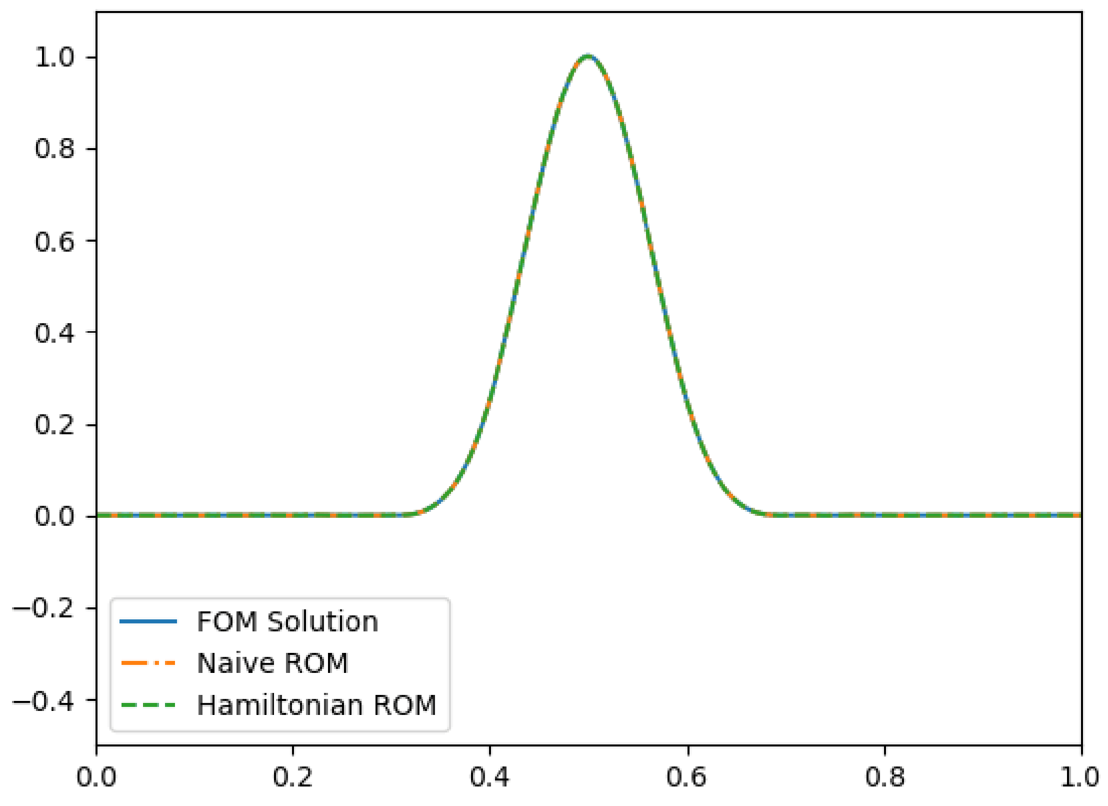
- Naïve Galerkin projection yields

$$\dot{\hat{\mathbf{y}}} = \mathbf{U}^\intercal \mathbf{J}_{2n} \nabla H(\tilde{\mathbf{y}}) \,.$$

  - NOT Hamiltonian,

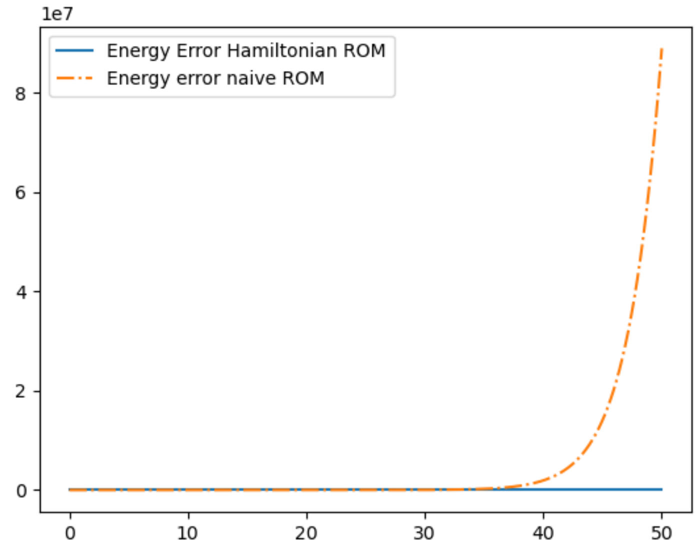
$$\mathbf{U}^\intercal \mathbf{L} \neq -\mathbf{L}^\intercal \mathbf{U} \,.$$

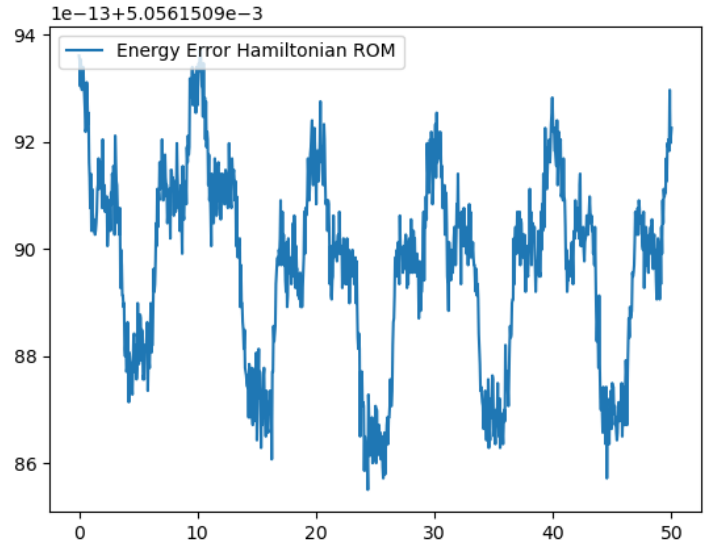
- Do we care?
  - Yes, predictive behavior is poor



What happened?

- Naïve Galerkin ROM is…
  - Not Hamiltonian (energy not conserved).
  - Not symplectic (Jacobi identity violated).
- Conversely, Hamiltonian ROM satisfies both.
  - Phase space volume never changes.
- How can we get this in our ROM?





Intrusive Hamiltonian ROMs

- One simple solution due to Y. Gong, Q. Wang, Z. Wang (2017):
  - Recall that $\nabla \hat{H}(\hat{\mathbf{x}}) = \tilde{\mathbf{x}}' \cdot \nabla H(\tilde{\mathbf{x}}) = \mathbf{U}^\intercal \nabla H(\tilde{\mathbf{x}})$.
- We want $\mathbf{U}^\intercal \mathbf{L} \nabla H(\tilde{\mathbf{x}}) = \hat{\mathbf{L}} \mathbf{U}^\intercal \nabla H(\tilde{\mathbf{x}}) = \hat{\mathbf{L}} \nabla \hat{H}(\hat{\mathbf{x}})$.
  - Implies the overdetermined system $\mathbf{U}^\intercal \mathbf{L} = \hat{\mathbf{L}} \mathbf{U}^\intercal$.
  - Solution is $\boxed{\hat{\mathbf{L}} = \mathbf{U}^\intercal \mathbf{L} \mathbf{U}}$.
- Yields low-dim Hamiltonian system $\dot{\hat{\mathbf{x}}} = \hat{\mathbf{L}}(\tilde{\mathbf{x}}) \nabla \hat{H}(\hat{\mathbf{x}})$.

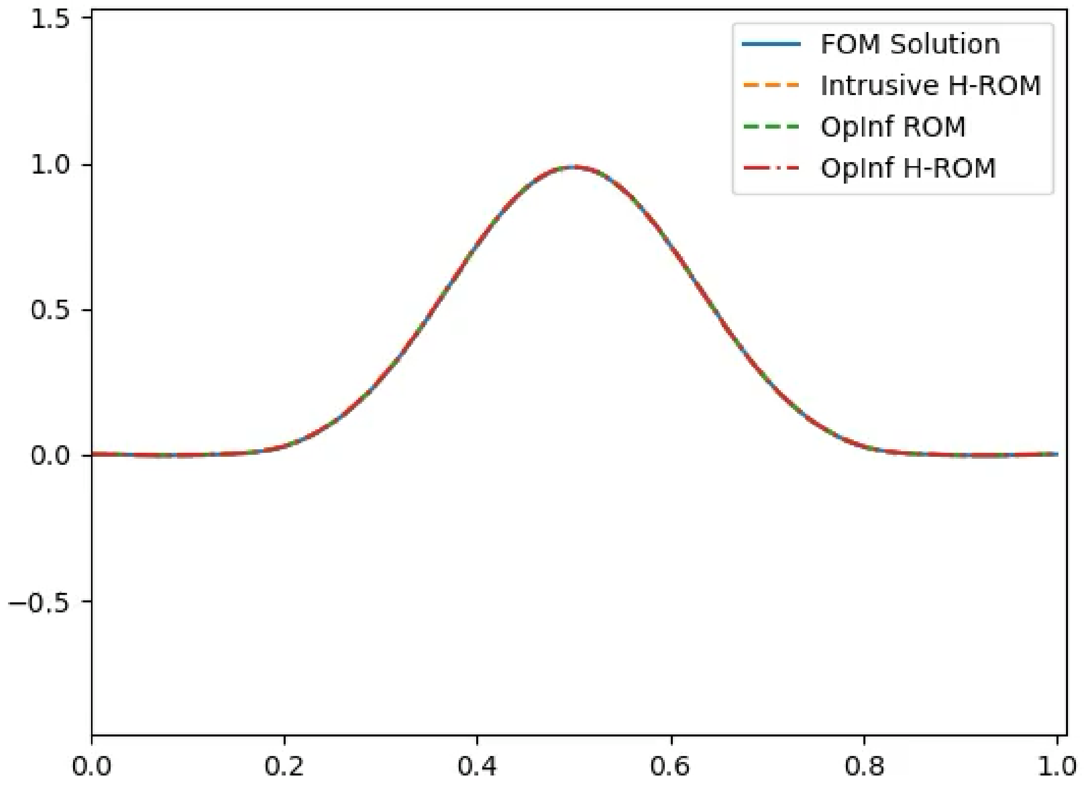
Nonintrusive Hamiltonian ROMs

- What happens if no access to FOM code? *Operator inference.*
- Partial solution for canonical systems (Sharma, Kramer, Wang 2022):
  - Postulate a reduced Hamiltonian $\hat{H}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}}) = \hat{\boldsymbol{q}}^\intercal \hat{\boldsymbol{A}}_{qq} \hat{\boldsymbol{q}} + \hat{\boldsymbol{p}}^\intercal \hat{\boldsymbol{A}}_{pp} \hat{\boldsymbol{p}}$.
  - Dynamical system becomes $\begin{pmatrix} \dot{\hat{\boldsymbol{q}}} \\ \dot{\hat{\boldsymbol{p}}} \end{pmatrix} = \begin{pmatrix} 0 & \boldsymbol{I} \\ -\boldsymbol{I} & 0 \end{pmatrix} \begin{pmatrix} \hat{\boldsymbol{A}}_{qq} & \boldsymbol{0} \\ \boldsymbol{0} & \hat{\boldsymbol{A}}_{pp} \end{pmatrix} \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{p} \end{pmatrix}$.
  - Infer

$$\hat{\boldsymbol{A}}_{qq} = \underset{\hat{\boldsymbol{A}} = \hat{\boldsymbol{A}}^\intercal}{\operatorname{argmin}} \left| \hat{\boldsymbol{X}}_{p,t} + \hat{\boldsymbol{A}} \hat{\boldsymbol{X}}_q \right|^2 \qquad \hat{\boldsymbol{A}}_{pp} = \underset{\hat{\boldsymbol{A}} = \hat{\boldsymbol{A}}^\intercal}{\operatorname{argmin}} \left| \hat{\boldsymbol{X}}_{q,t} - \hat{\boldsymbol{A}} \hat{\boldsymbol{X}}_p \right|^2$$

Does it work?

- Yeah! But…
  - Relies on $\boldsymbol{U}^\intercal \boldsymbol{J} = \boldsymbol{J}_r \boldsymbol{U}^\intercal$.
  - Needs a block-diagonal $\nabla \hat{H}$
- How to extend to more general systems?



Hamiltonian Operator Inference

- Recognize special case of more general OpInf procedure:
  - Can solve $\underset{\hat{\boldsymbol{L}} \text{ or } \hat{\boldsymbol{A}}}{\operatorname{argmin}} \left| \hat{\boldsymbol{X}}_t - \hat{\boldsymbol{L}}\hat{\boldsymbol{A}}\hat{\boldsymbol{X}} \right|^2, \quad \hat{\boldsymbol{L}}^\intercal = -\hat{\boldsymbol{L}}, \hat{\boldsymbol{A}}^\intercal = \hat{\boldsymbol{A}}.$
- If $\boldsymbol{L}$ is known, this is *"canonical" inference!*
- If ∇H is known, this is *noncanonical inference.*

KdV Equation

- Consider solving $u_t = \alpha u u_x + \rho u_x + \gamma u_{xxx},$ $[-L, L] \times [0, T]$
- Recast as $u_t = \mathcal{D} \frac{\delta \mathcal{H}}{\delta u},$ $\mathcal{H} = \int_0^L \left(\frac{\alpha}{6} u^3 + \frac{\rho}{2} u^2 - \frac{\nu}{2} u_x^2 \right) dx.$ $\mathcal{D} = \partial_x$
- Discretizing with periodic BCs yields

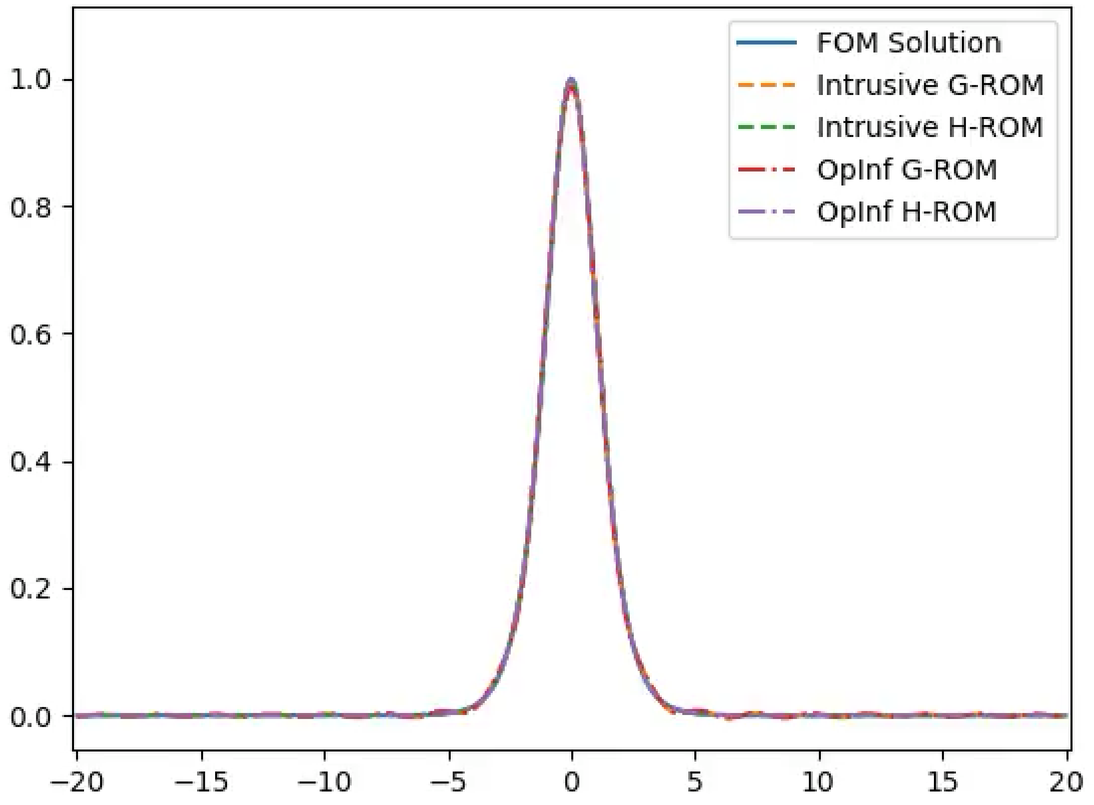
$$\frac{d\mathbf{u}}{dt} = \mathbf{A} \nabla_{\mathbf{u}} H(\mathbf{u}) = \mathbf{A} \left(\frac{\alpha}{2} \mathbf{u}^2 + \rho \mathbf{u} + \nu \mathbf{B} \mathbf{u} \right)$$

$$\mathbf{A} = \frac{1}{2\Delta x} \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & -1 \\ -1 & 0 & 1 & 0 & \cdots & 0 \\ & & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & -1 & 0 & 1 \\ 1 & \cdots & 0 & 0 & -1 & 0 \end{pmatrix}, \quad \mathbf{B} = \frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 & 0 & 0 & \cdots & 1 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ & & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & 1 & -2 & 1 \\ 1 & \cdots & 0 & 0 & 1 & -2 \end{pmatrix}$$

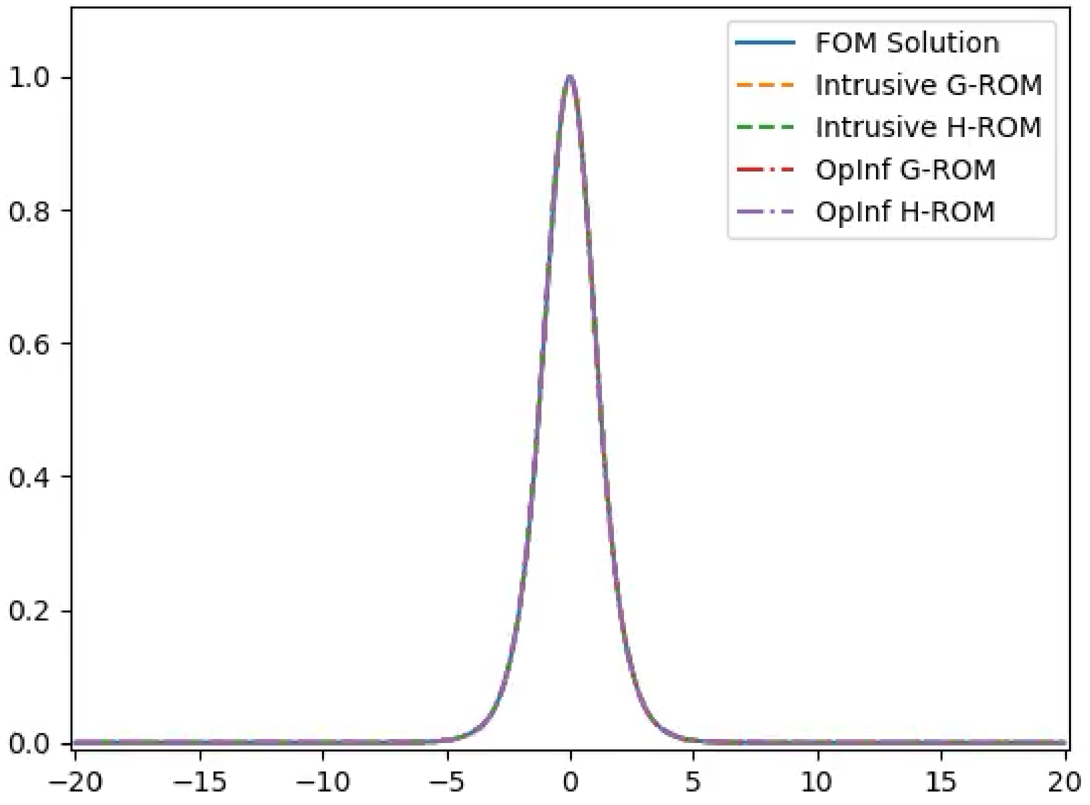
$$u_0(x) = \operatorname{sech}^2 \left(\frac{x}{\sqrt{2}} \right)$$

  - A = L is non-canonical!

KdV Equation

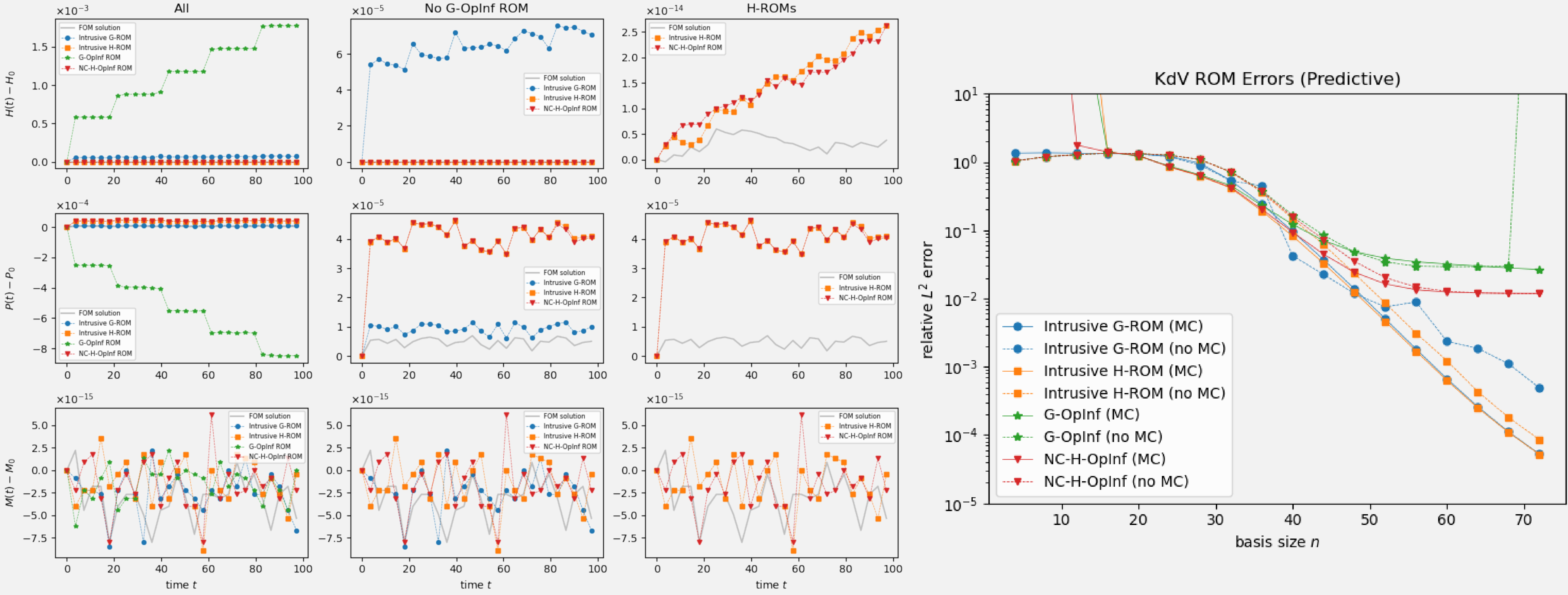


N = 500, n=36



N = 500, n=48

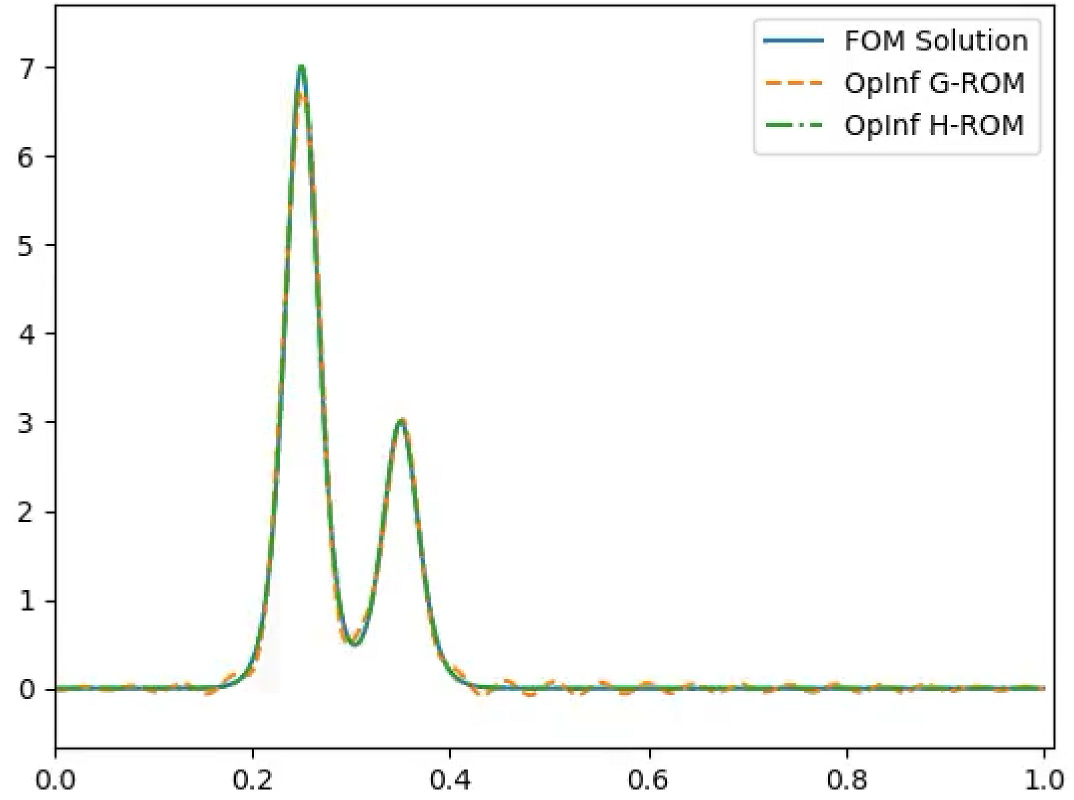
KdV Equation



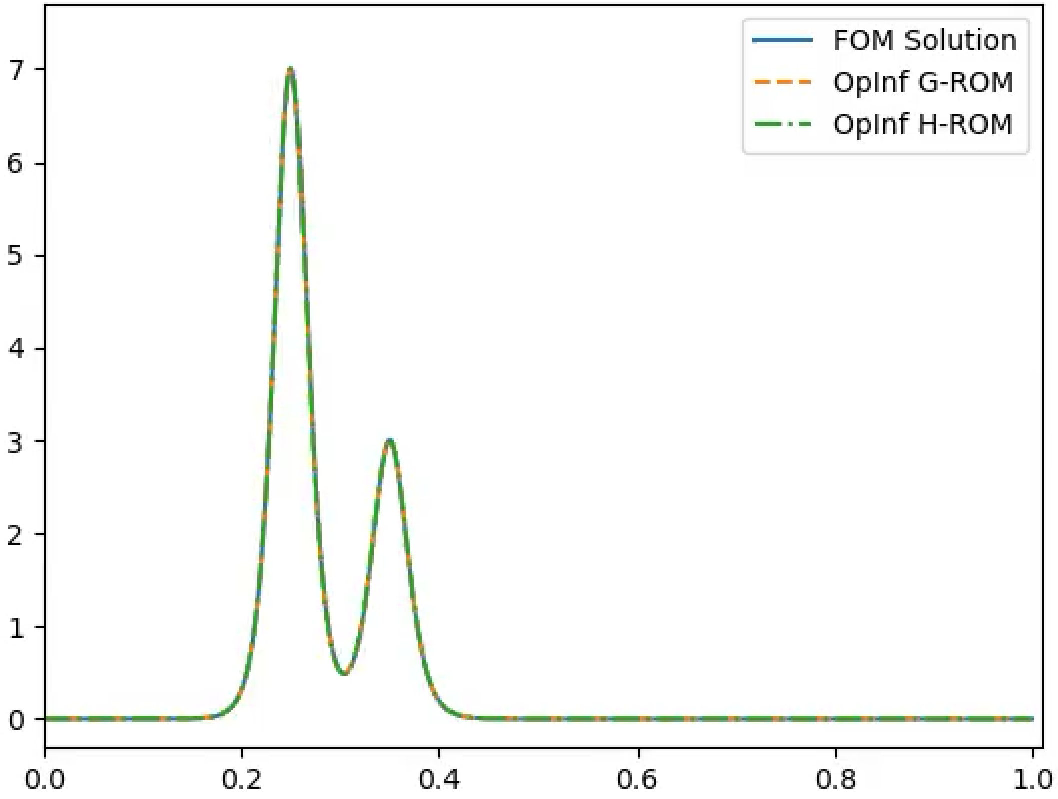
BBM Equation

- Benjamin-Bona-Mahoney equation: $\dot{x} = \alpha x_s + \beta x x_s - \gamma \dot{x}_{ss}.$
- Hamiltonian: $H(x) = \frac{1}{2}\int_0^{\ell} \alpha x^2 + \frac{\beta}{3} x^3 \, ds,$
- Poisson structure: $L = -\left(1 - \partial_s^2\right)^{-1} \partial_s,$
- Intrusive H-ROM not feasible
    - Can we still get a good OpInf H-ROM?

BBM Equation

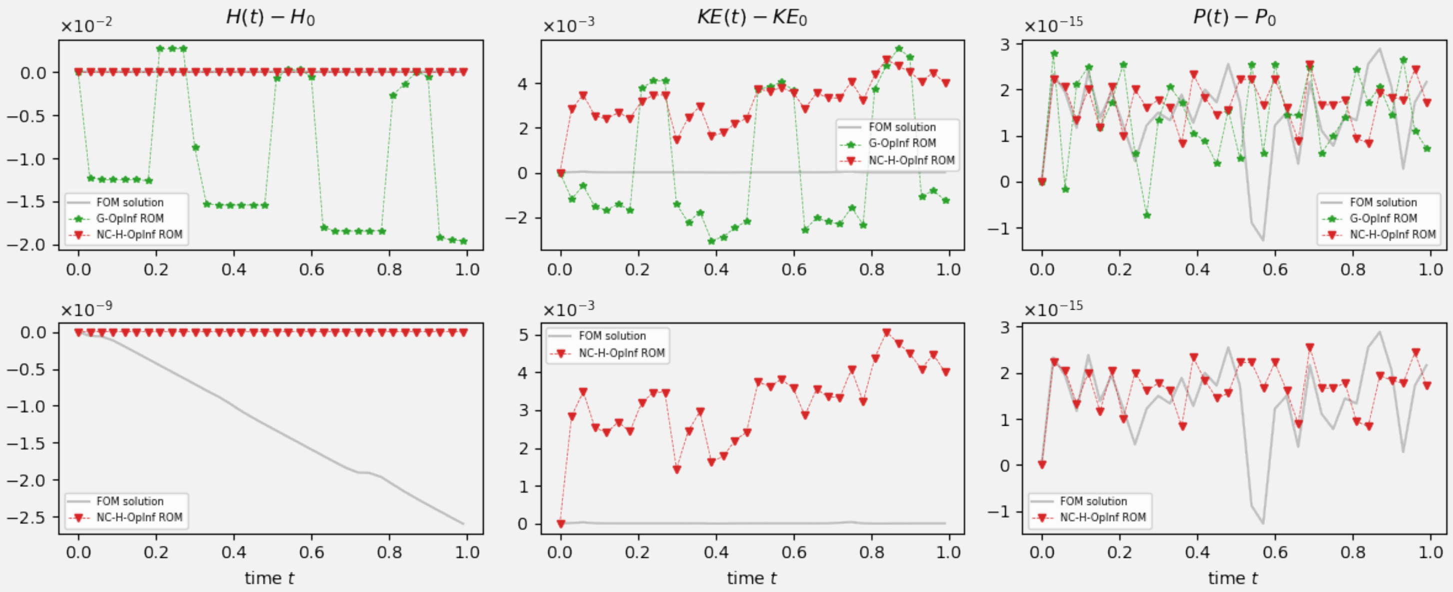


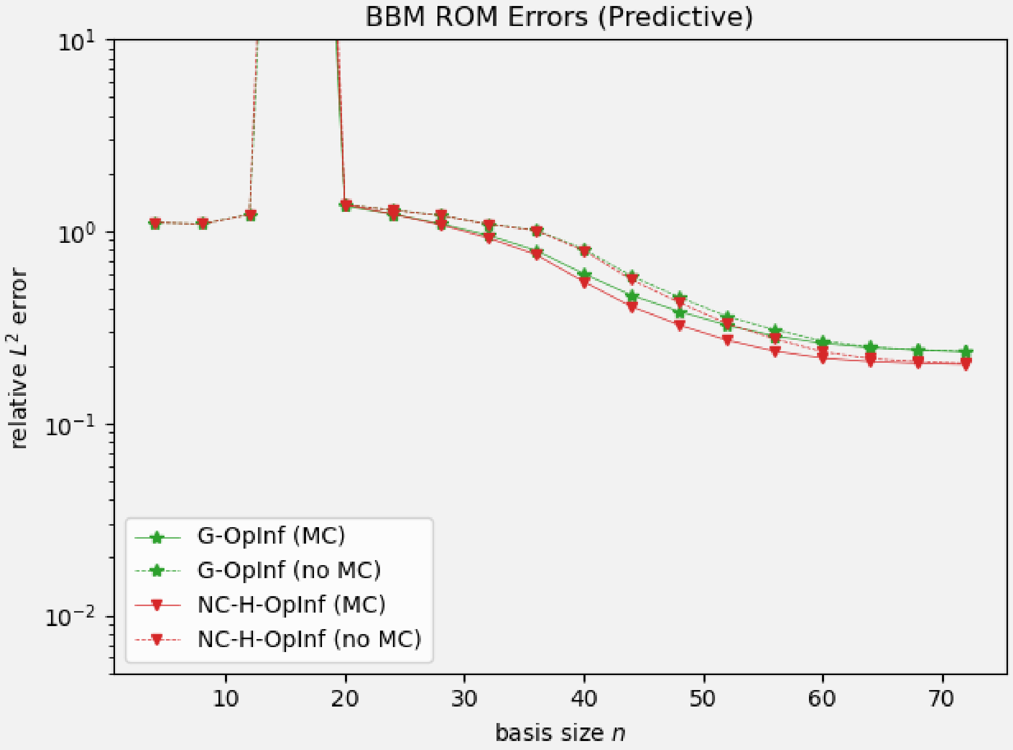
N = 1024, n=36



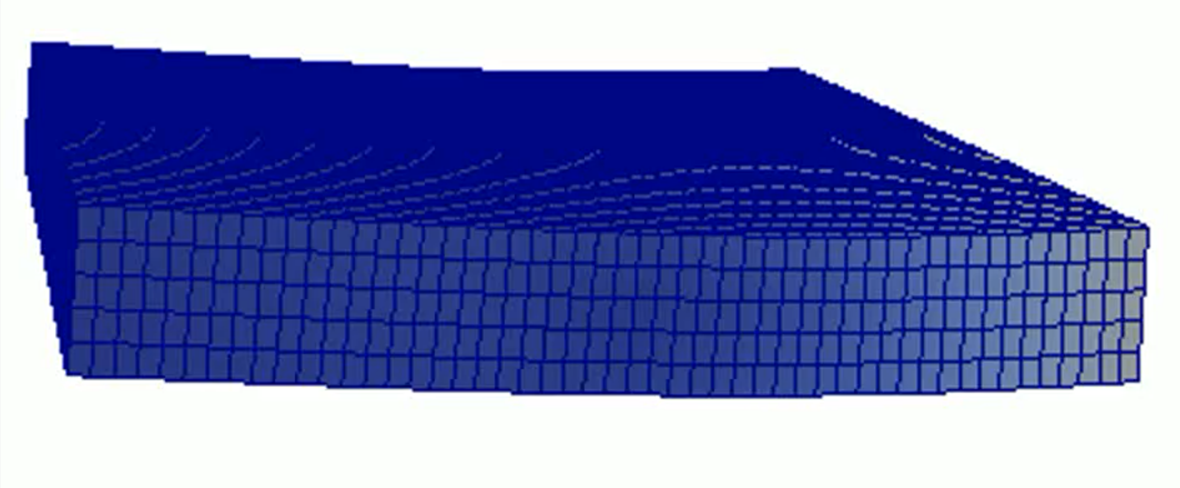
N = 1024, n=72

BBM Equation





Problem solved?



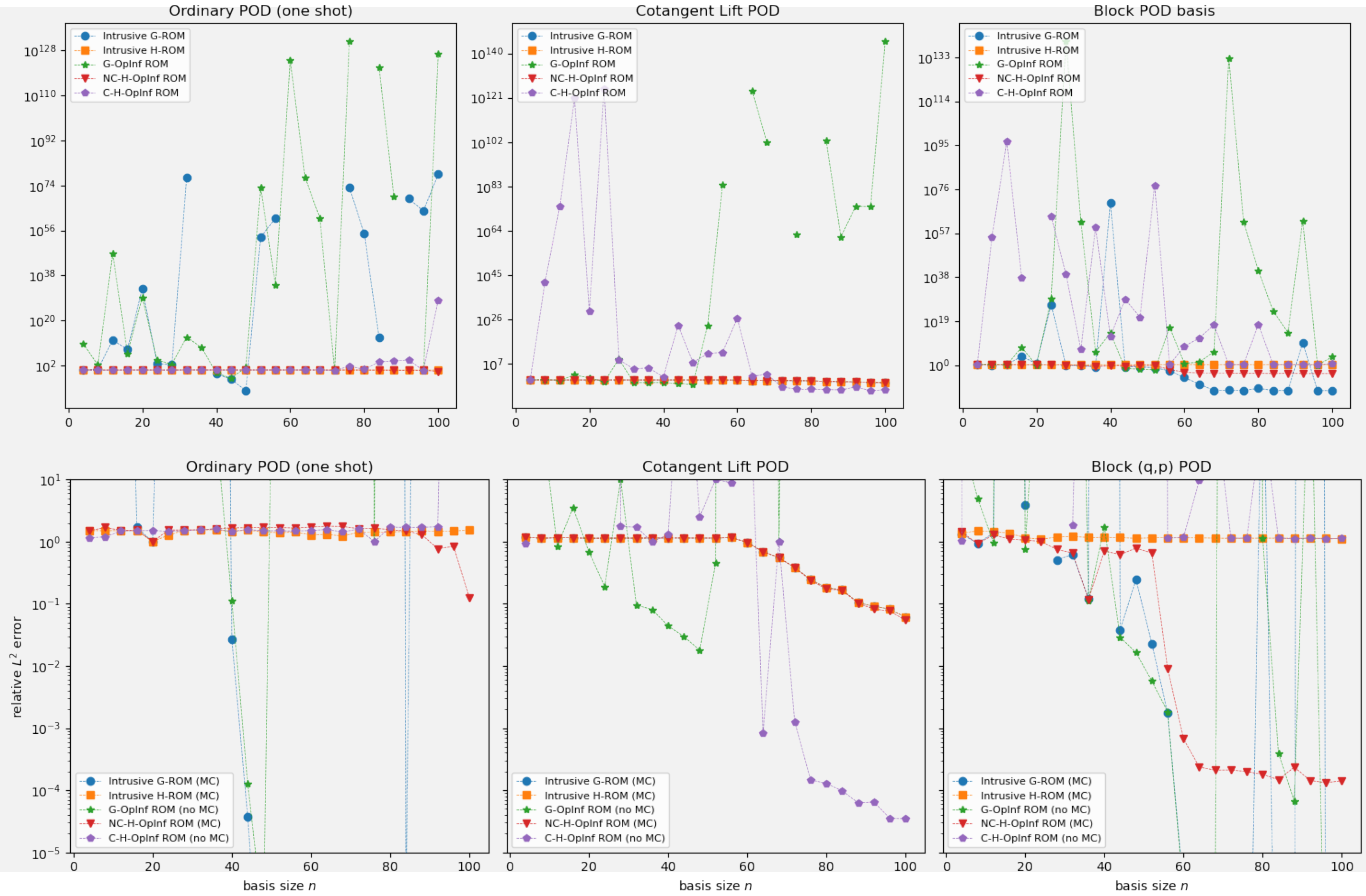
- Only in simple cases.
  - Issues when scaling up…
- Consider a 3D linear elastic system:

$$\mathbf{M}\ddot{\mathbf{q}} + \mathbf{K}\mathbf{q} = \mathbf{0}\,.$$

$$H(\boldsymbol{q},\boldsymbol{p}) = \frac{1}{2}\left(\boldsymbol{q}^\intercal \boldsymbol{K}\boldsymbol{q} + \boldsymbol{p}^\intercal \boldsymbol{M}^{-1}\boldsymbol{p}\right)$$

- Equivalent Hamiltonian form: $\dot{\boldsymbol{x}} = \begin{pmatrix}\dot{\boldsymbol{q}}\\ \dot{\boldsymbol{p}}\end{pmatrix} = \begin{pmatrix}0 & \boldsymbol{I}\\ -\boldsymbol{I} & 0\end{pmatrix}\begin{pmatrix}\boldsymbol{K} & 0\\ 0 & \boldsymbol{M}^{-1}\end{pmatrix}\begin{pmatrix}\boldsymbol{q}\\ \boldsymbol{p}\end{pmatrix} = \boldsymbol{J}\boldsymbol{A}\boldsymbol{x},$

Good news and bad



Thank you!

Contact: adgrube@sandia.gov

References:

A. Gruber, M. Gunzburger, L. Ju, Z. Wang, "Energetically Consistent Model Reduction for Metriplectic Systems", CMAME, 2023

A. Gruber, I. Tezaur, M. Gunzburger, "Canonical and Noncanonical Hamiltonian Operator Inference", (coming soon!)

Codes:
https://github.com/agrubertx/metriplectic_POD-ROM
https://github.com/ikalash/HamiltonianOpInf