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Property-preserving model reduction for conservative and dissipative systems

Anthony Gruber

Center for Computing Research, Sandia National Laboratories, Albuquerque, NM

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Full-Order Model

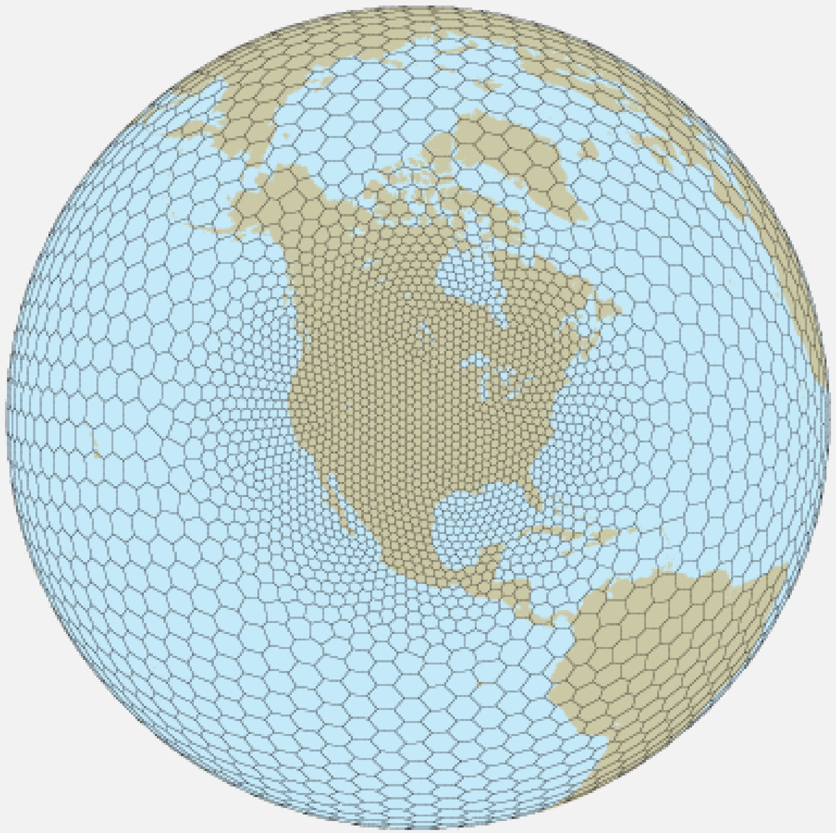
- Consider state variable $\mathbf{x}(t, \boldsymbol{\mu}) \in \mathbb{R}^N$.
  - *N* ranges from “large” to “very large” (10^{6+} not uncommon).
  - $\boldsymbol{\mu}$ is vector of parameters.
- Dynamics take the form

$$\dot{\mathbf{x}}(t, \boldsymbol{\mu}) = \mathbf{A}\mathbf{x}(t, \boldsymbol{\mu}) + \mathbf{f}\left(\mathbf{x}(t, \mu)\right).$$

  - Can be expensive to solve. How to reduce cost?

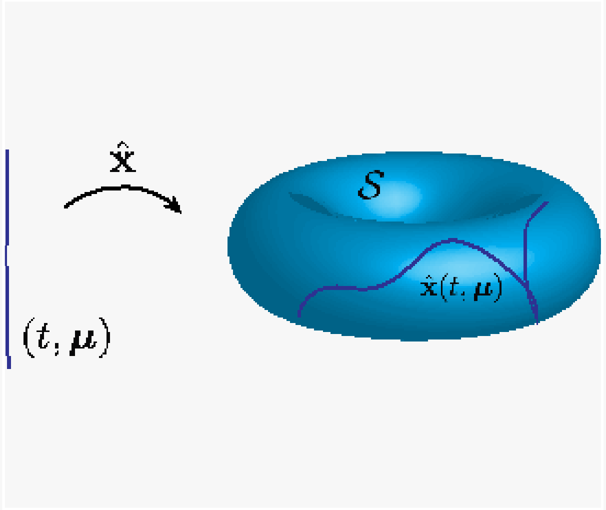
Reduced-Order Models

- High-fidelity PDE simulations are **expensive.**
  - semi-discretization blows up dimensionality.
- Good results possible without solving full PDE?
- Standard is to **encode -> solve -> decode.**
  - Linear: POD, RBM, etc.
  - Nonlinear: kernel methods, neural networks, etc.



https://mpas-dev.github.io/atmosphere/atmosphere.html

Outline



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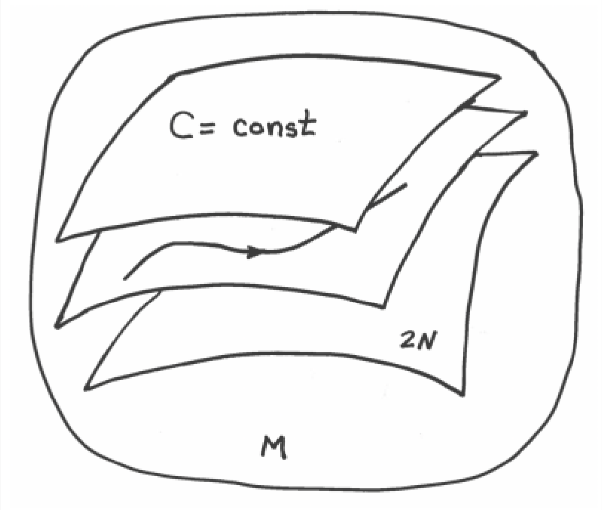
Introduction to Model Reduction



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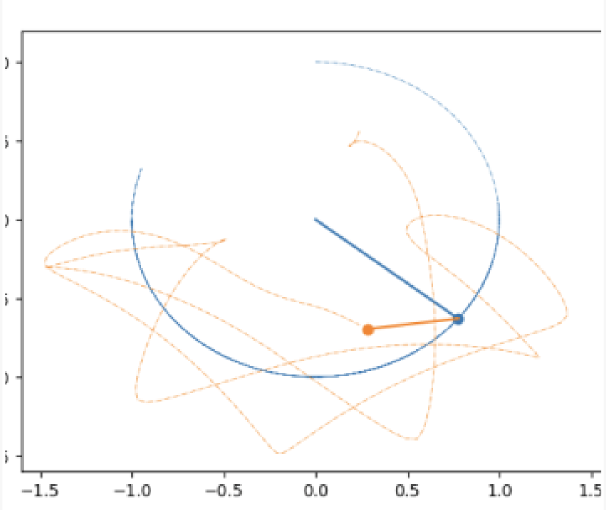
Hamiltonian Model Reduction



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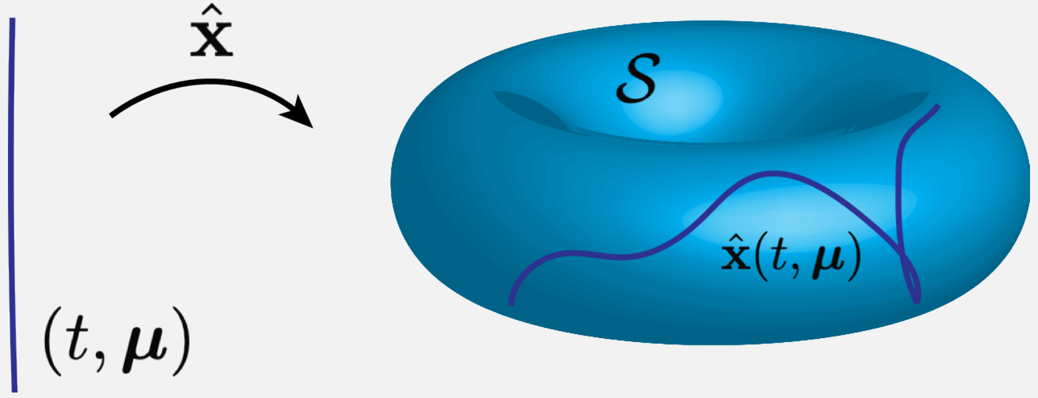
Metriplectic Model Reduction

- Joint work with **Max Gunzburger (UT Austin), Lili Ju (U of SC), Zhu Wang (U of SC),** and **Irina Tezaur (Sandia CA).**

Idea Behind ROM

- Do we really need all 10^6 dimensions?
  - No, if $(t, \boldsymbol{\mu}) \mapsto \boldsymbol{x}(t, \boldsymbol{\mu})$ is unique.
- $\mathcal{S} = \{\boldsymbol{x}(t, \boldsymbol{\mu}) \mid t \in [0, T],\ \boldsymbol{\mu} \in D\} \subset \mathbb{R}^N$, solution manifold.
  - $(n_\mu + 1)$ dimensions enough for loss-less representation of $\mathcal{S}$.
- How can we approximate $\mathcal{S}$ efficiently?



Proper Orthogonal Decomposition

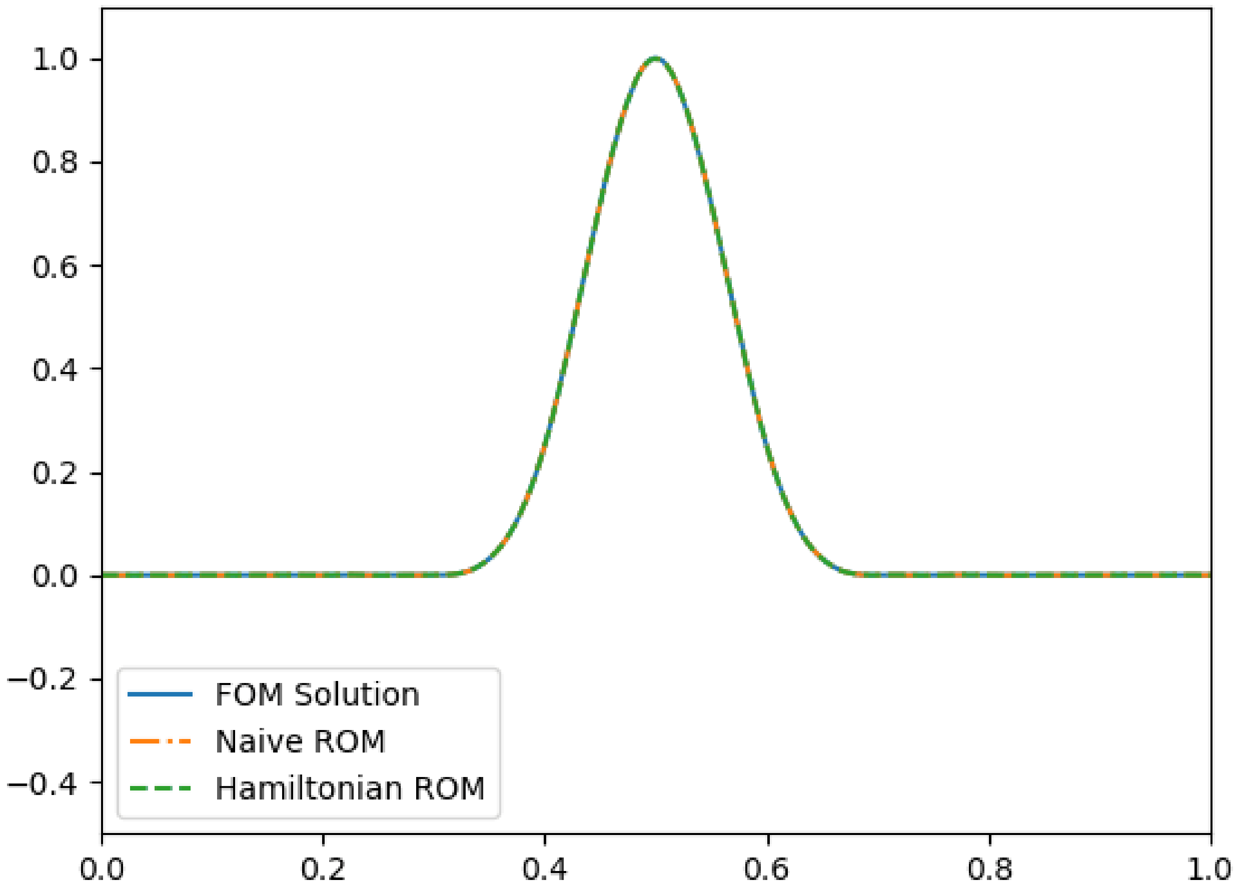
- Do PCA on solution snapshots $\boldsymbol{X} = \boldsymbol{x}(t_j, \boldsymbol{\mu}_j),\ 1 \leq j \leq N_t$.
  - Yields $\mathbf{X} \approx \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\intercal$, Galerkin projection $\boxed{\tilde{\mathbf{x}} = \mathbf{U}\hat{\mathbf{x}}}$.
- Orthogonality of POD basis $\mathbf{U}$ 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*.

Does this work?

- Trained on one period
    - Tested on five



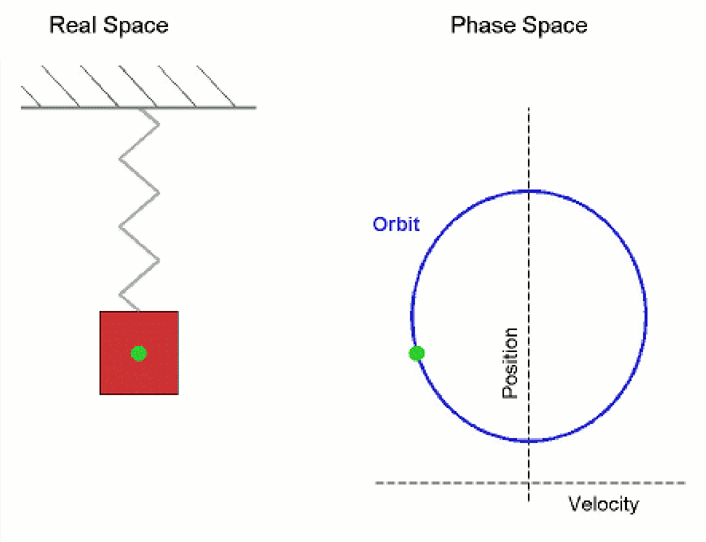
Hamiltonian Systems

- 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) Hamiltonian Systems

GIFs courtesy of Wikipedia under Creative Commons license



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

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

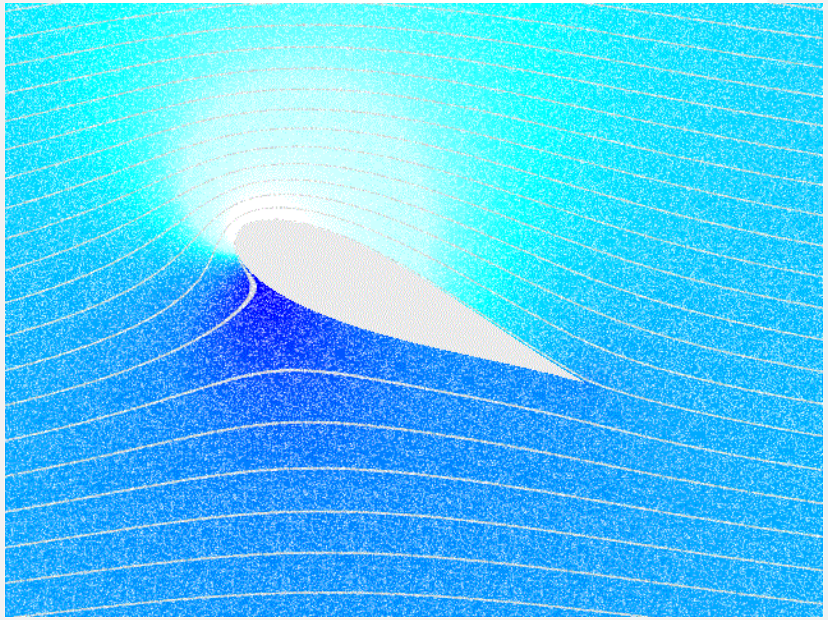
$$p = m\dot{x}, \quad q = m\sqrt{\frac{k}{m}}x$$

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

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

  - Warning! Vorticity is the Hamiltonian variable!

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



What about ROM?

- Naïve Galerkin projection yields $\dot{\hat{\mathbf{x}}} = \mathbf{U}^\intercal \mathbf{L} \nabla H(\tilde{\mathbf{x}})$.
  - Not Hamiltonian, $\mathbf{U}^\intercal \mathbf{L} \neq -\mathbf{L}^\intercal \mathbf{U}$.
- One 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 $\boxed{\hat{\mathbf{L}} = \mathbf{U}^\intercal \mathbf{L} \mathbf{U}}$, (antisymmetry is obviously inherited).

Hamiltonian ROM

- Energy conservation is retained:

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

- Can prove convergence to FOM solution with increasing POD basis.

- Need a symplectic time integrator (many choices available).
  - For "easy" nonlinearities, AVF is a good choice.

$$\frac{\mathbf{x}^{k+1} - \mathbf{x}^k}{\Delta t} = \int_0^1 \mathbf{L} \nabla H \left(t\mathbf{x}^{k+1} + (1-t)\mathbf{x}^k \right) \, dt$$

Nonintrusive Hamiltonian ROMs

- What happens if no access to FOM code? *Operator inference.*

- Partial solution for canonical systems (Sharma, Kramer, Wang 2022):

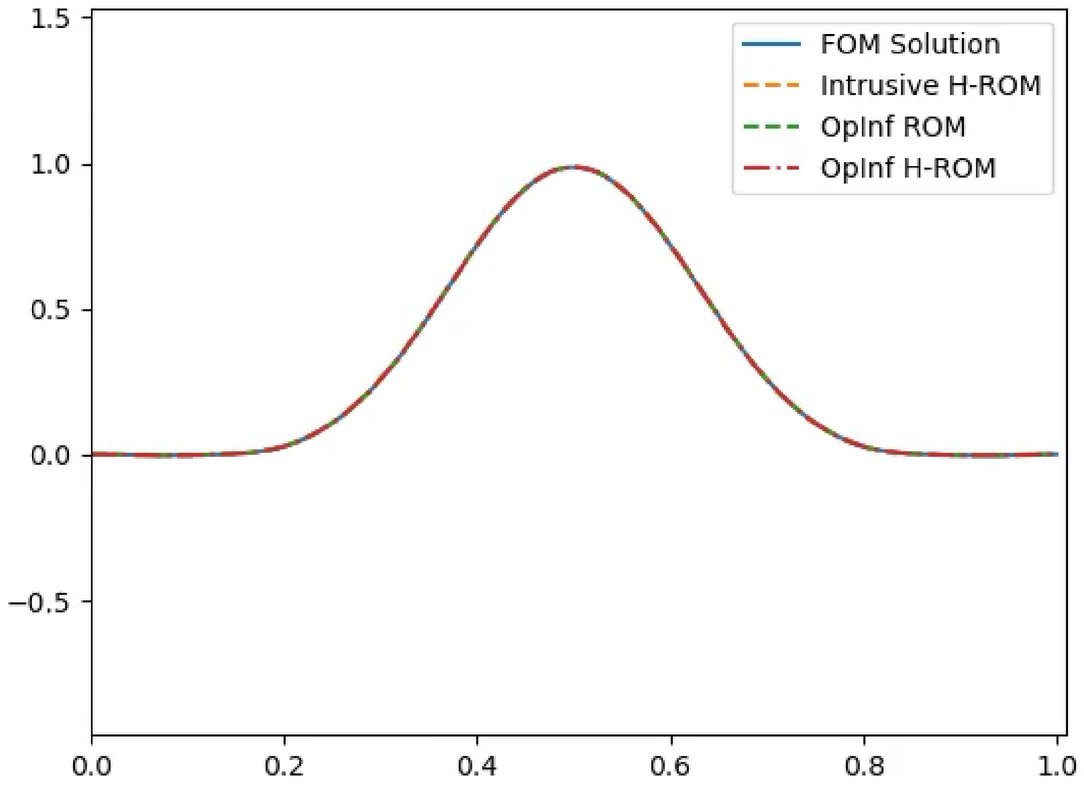
  - Postulate a reduced Hamiltonian $\hat{H}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}}) = \hat{\boldsymbol{q}}^\intercal \hat{\boldsymbol{A}}_{qq} \hat{\boldsymbol{q}} + \hat{\boldsymbol{p}}^\intercal \hat{\boldsymbol{A}}_{pp} \hat{\boldsymbol{p}}$.

  - 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:
  - Joint w. Irina Tezaur (Sandia CA)
  - 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.*

Hamiltonian Operator Inference

- Need to solve minimization

$$\underset{\mathbf{D}\in\mathbb{R}^{N\times N}}{\operatorname{argmin}} \left(\left|\mathbf{C} - \mathbf{A}\left(\mathbf{D} \pm \mathbf{D}^\intercal\right)\mathbf{B}\right|^2 + \eta\left|\mathbf{D}\right|^2 \right),$$

- Boils down to *unconstrained* linear system:

$$\left(\left(\mathbf{A}^\intercal\mathbf{A} \mathbin{\bar{\oplus}} \mathbf{B}\mathbf{B}^\intercal\right)\left(\mathbf{I} \pm \mathbf{K}\right) + \eta\mathbf{I}\right)\operatorname{vec}\mathbf{D} = \operatorname{vec}\left(\mathbf{A}^\intercal\mathbf{C}\mathbf{B}^\intercal \pm \mathbf{B}\mathbf{C}^\intercal\mathbf{A}\right),$$

where $\mathbf{A} \mathbin{\bar{\oplus}} \mathbf{B} = \mathbf{A}\otimes\mathbf{B} + \mathbf{B}\otimes\mathbf{A}$, $\operatorname{vec}\mathbf{D}^\intercal = \mathbf{K}\operatorname{vec}\mathbf{D}$.

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

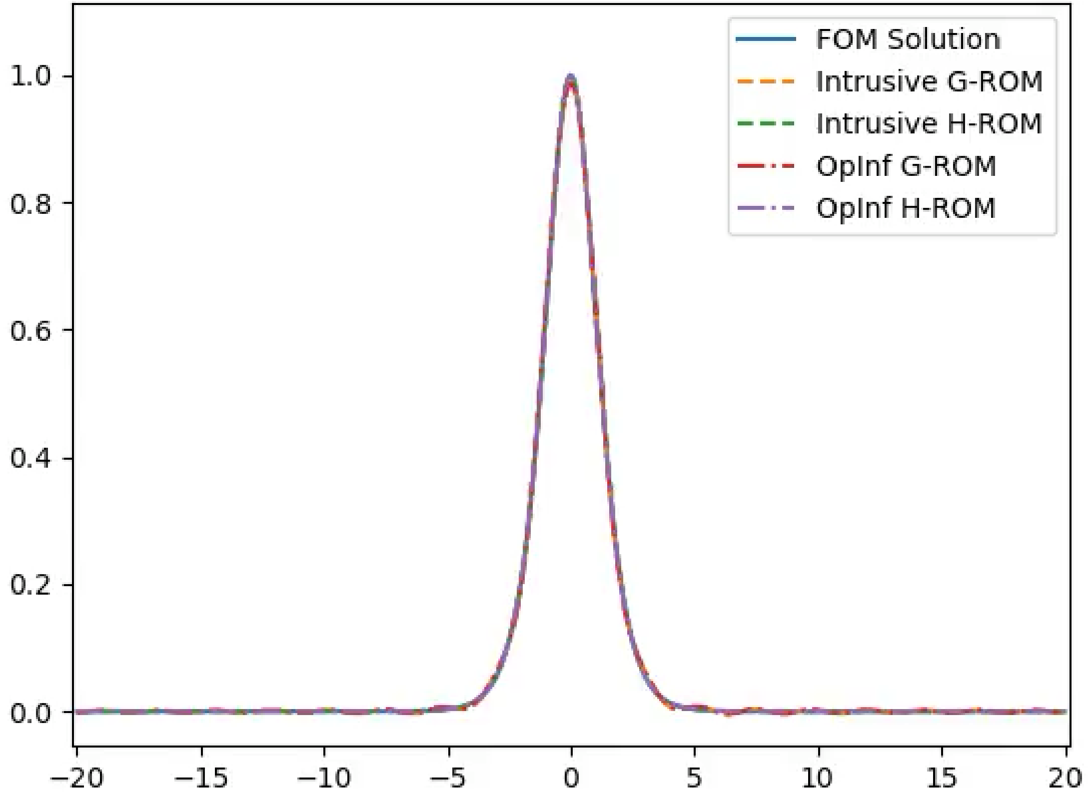
$$\begin{aligned}\frac{d\mathbf{u}}{dt} &= \mathbf{A}\nabla_{\mathbf{u}} H(\mathbf{u}) \\ &= \mathbf{A}\left(\frac{\alpha}{2}\mathbf{u}^2 + \rho\mathbf{u} + \nu\mathbf{B}\mathbf{u}\right)\end{aligned}$$

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

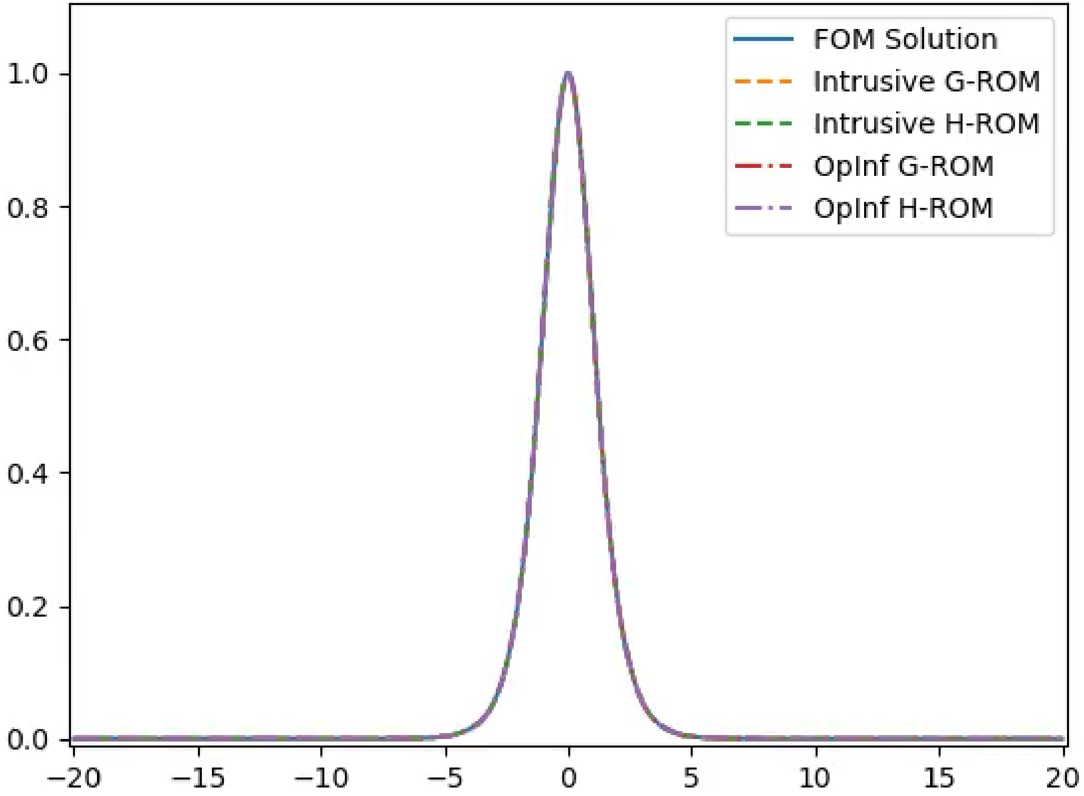
$$u_0(x) = \operatorname{sech}^2\left(\frac{x}{\sqrt{2}}\right)$$

  - A = L is non-canonical!

KdV Equation

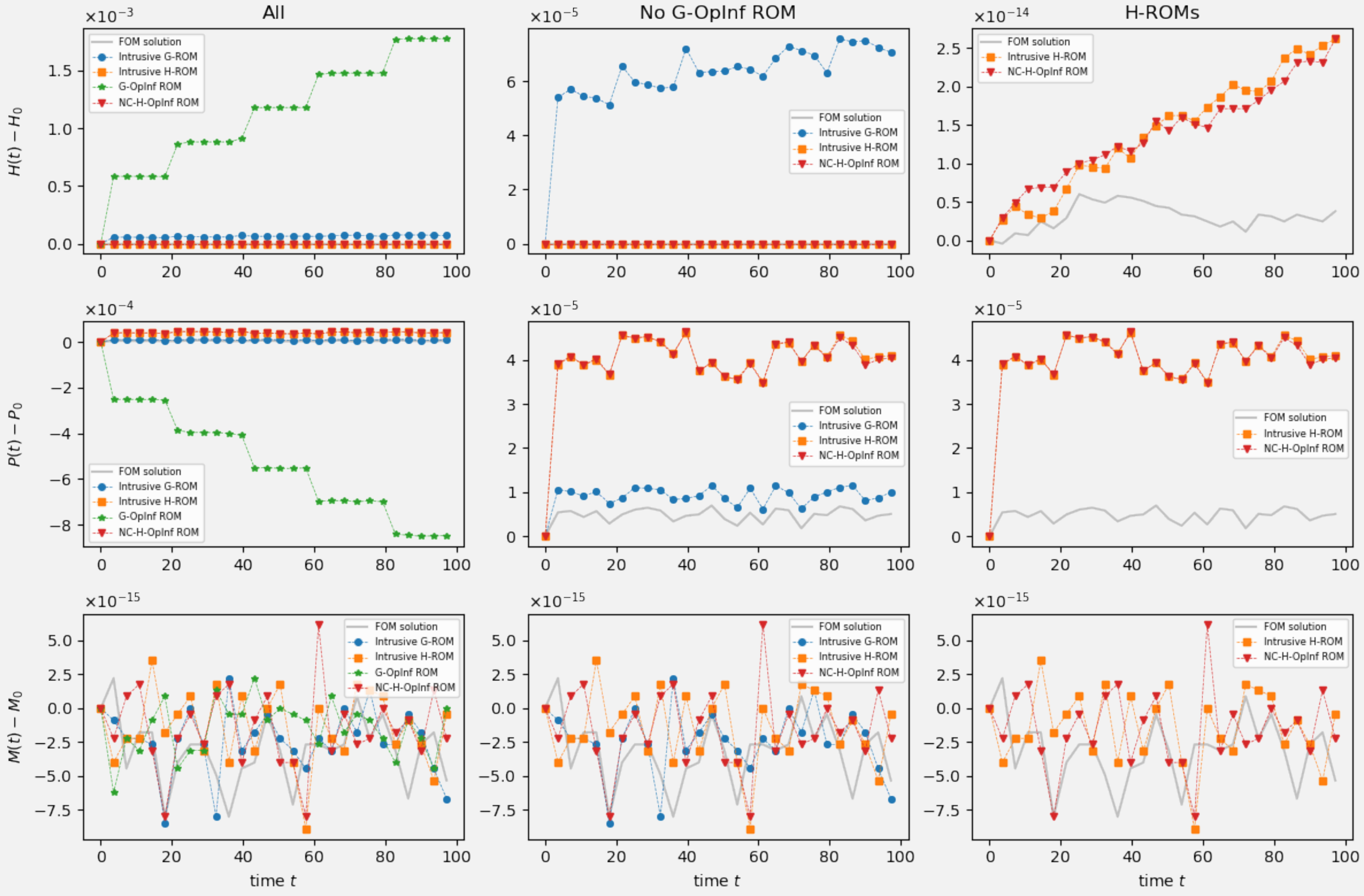


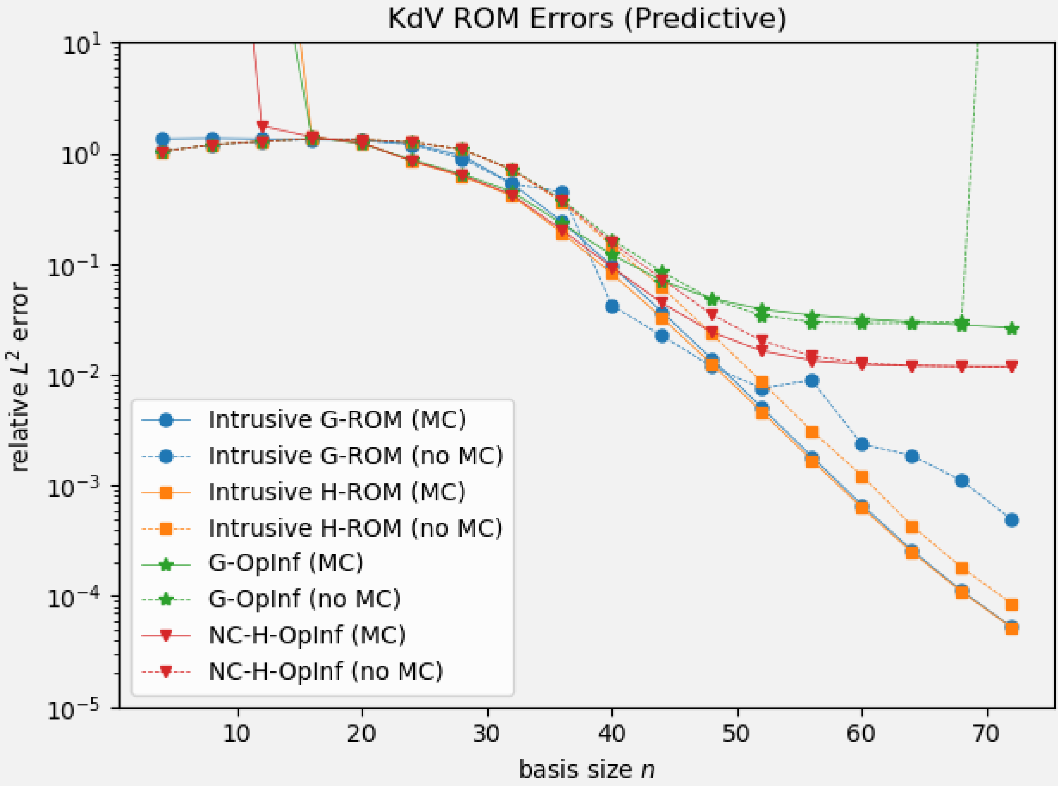
N = 500, n=36



N = 500, n=48

KdV Equation





Convergence with increasing data

- If $\lim_{n\to N} \left|\left(\mathbf{I} - \mathbf{U}\mathbf{U}^\intercal\right)\mathbf{x}\right| = 0,\ \forall \mathbf{x}$,

  $\lim_{\Delta t \to 0} \max_i \left|\mathbf{x}_t(t_i) - \dot{\mathbf{x}}(t_i)\right| = 0$,

  $\mathbf{X}, H(\mathbf{X})$ have maximal rank.

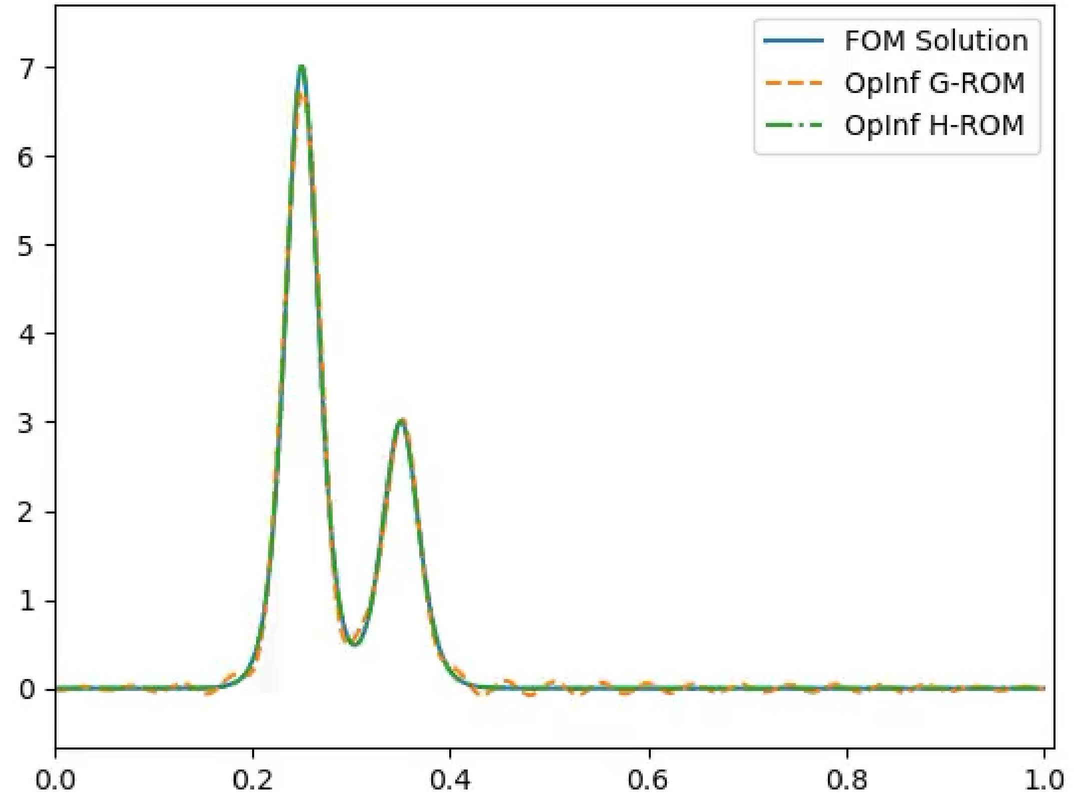
- *Theorem:* $\hat{\mathbf{L}} \to \mathbf{U}^\intercal \mathbf{L} \mathbf{U}$, $\hat{\mathbf{A}} \to \mathbf{U}^\intercal \mathbf{A} \mathbf{U}$

  as $n \to N$ and $\Delta t \to 0$.

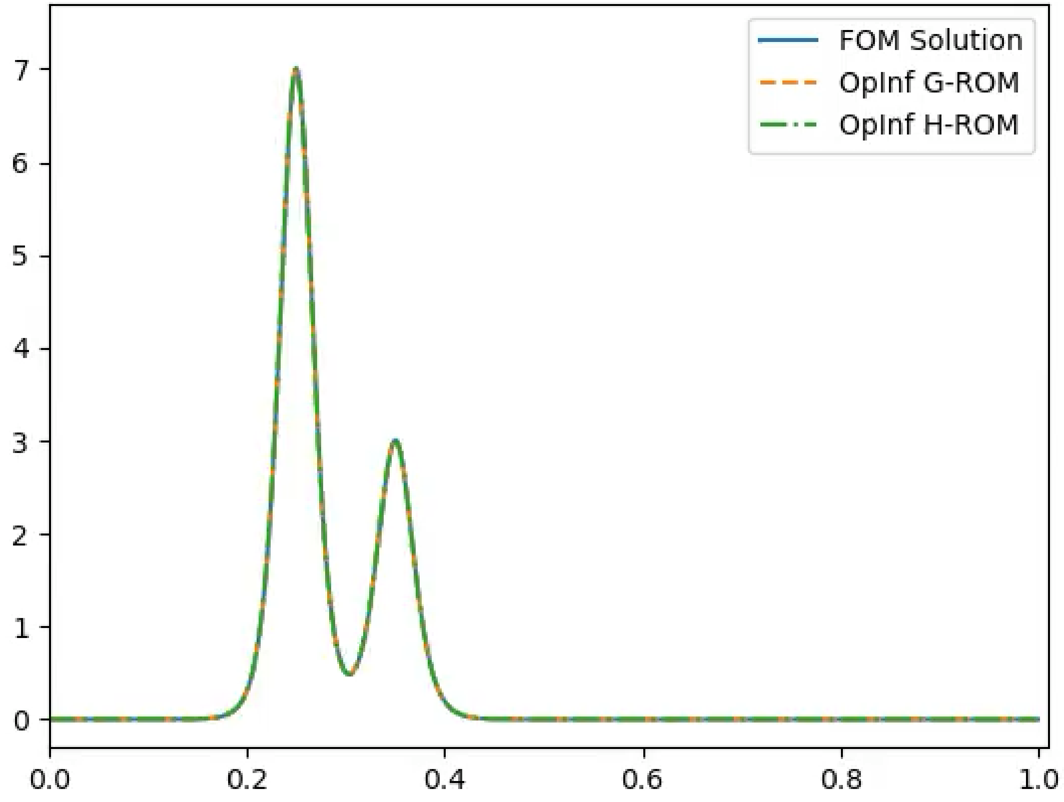
BBM Equation

- 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

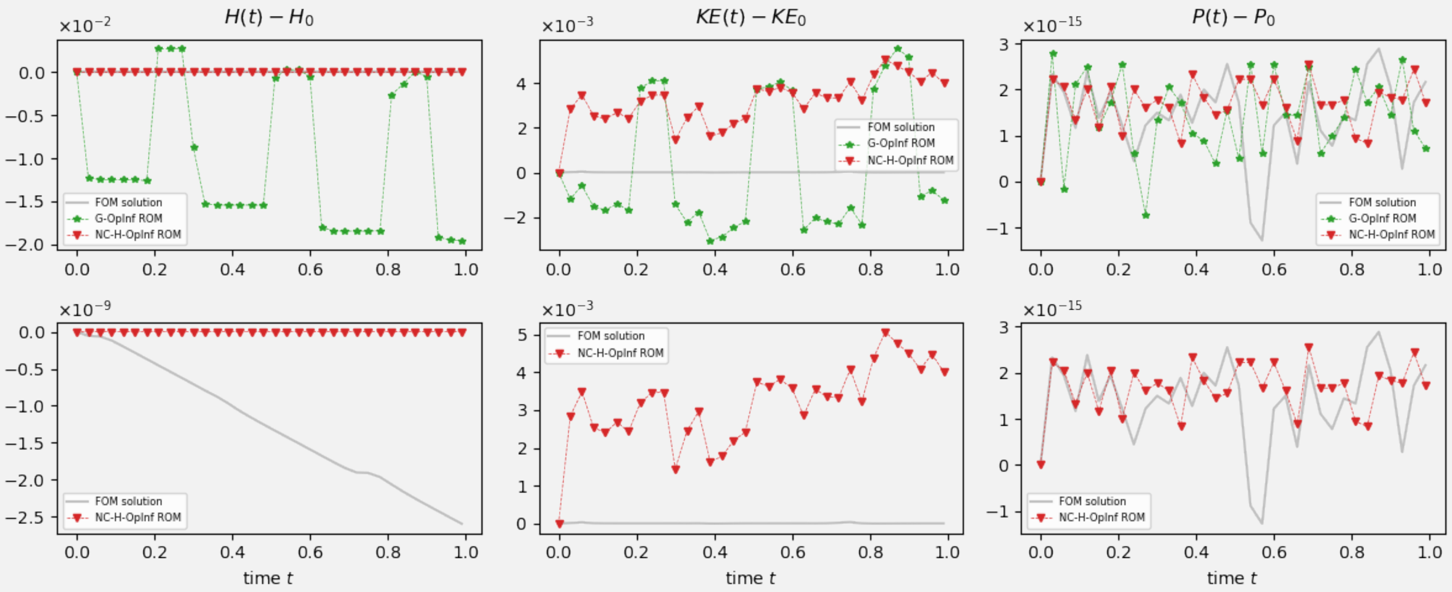


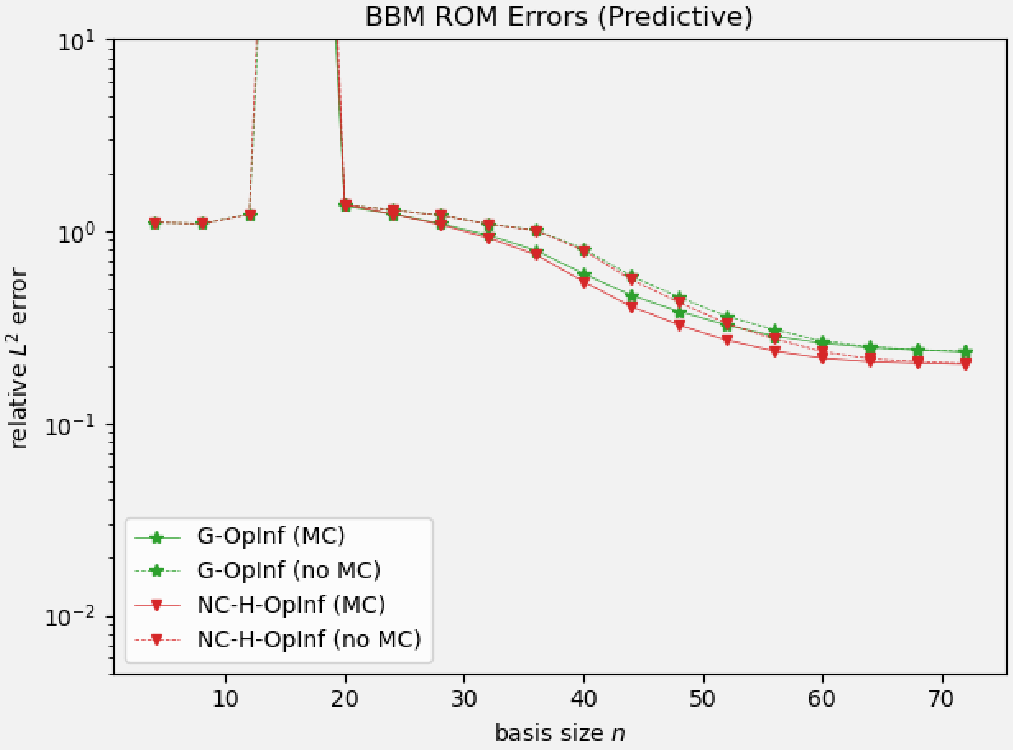
N = 1024, n=36



N = 1024, n=72

BBM Equation

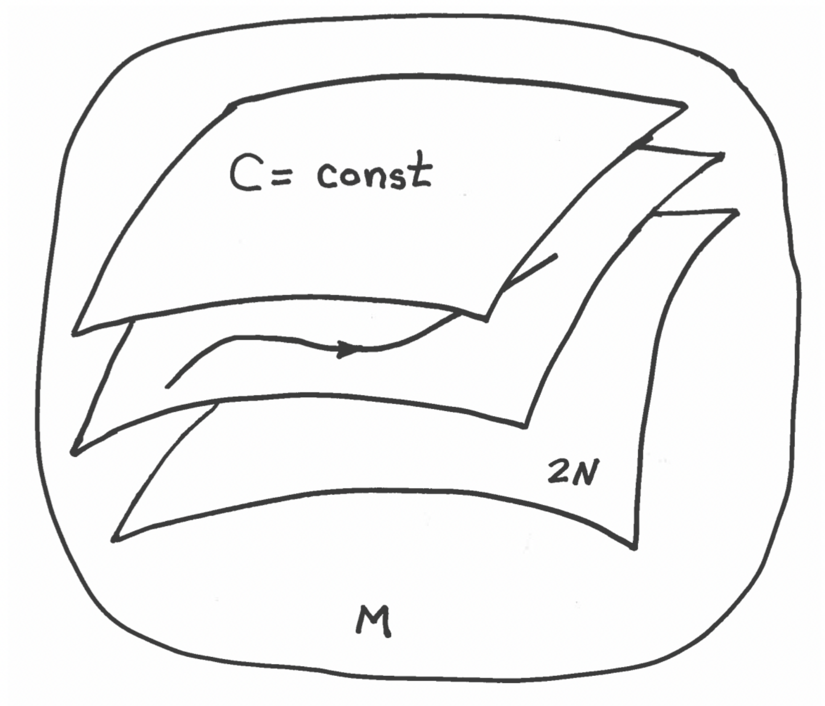




Beyond Hamiltonian systems

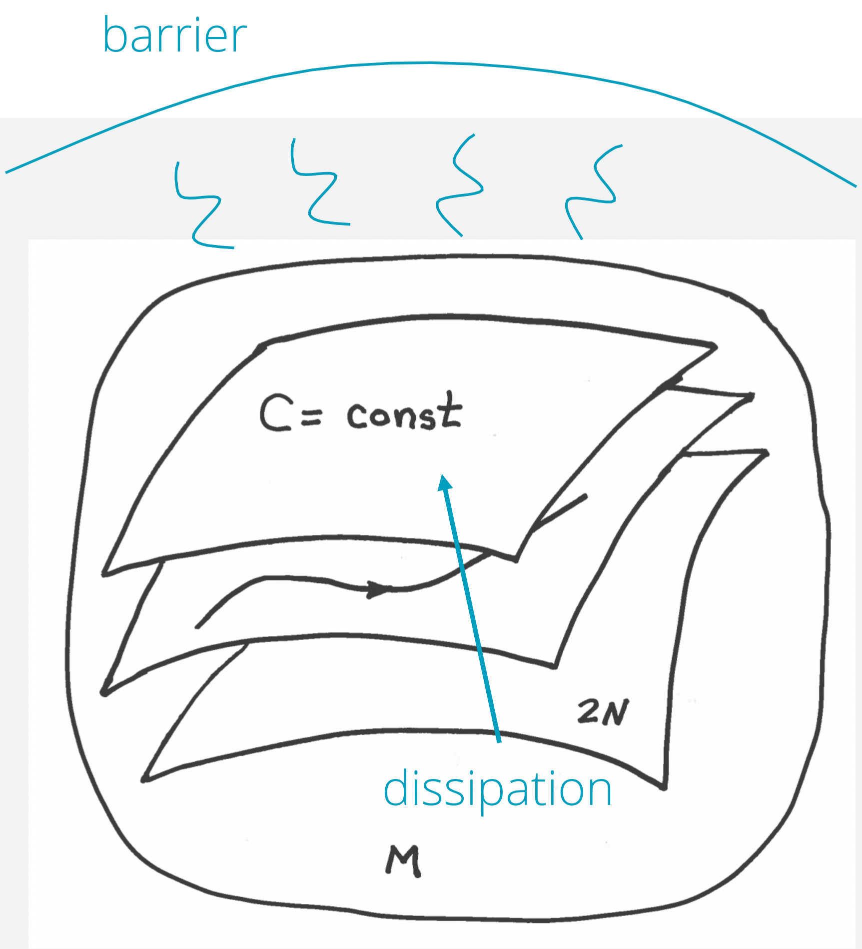
- Generalizes first law of thermodynamics.
    - Only useful for conservative systems!
- What about, e.g., dissipation?
    - Need *two* laws….
- Recall Casimir invariants: $\{\cdot, C\} = \mathbf{L}\nabla C = \mathbf{0}$.
    - Casimirs are potential entropy functions.

Illustration courtesy of P. J. Morrison



Beyond Hamiltonian systems

- Notice, $H' = H + \lambda^i C_i$ generates same dynamics as H.
    - But relaxes to different equilibria!
- Can we maintain a complete picture of the dynamics?
    - Choose $S = C$ for some Casimir C.
- Analogue of *isolated* systems in thermodynamics.
    - Examples: Boltzmann equation, Vlasov with collisions.



Metriplectic Systems

- Consider a system $\dot{\mathbf{x}} = \{\mathbf{x}, E\} + [\mathbf{x}, S] = \mathbf{L}\nabla E + \mathbf{M}\nabla S$.
    - Hamiltonian + Gradient: $\mathbf{L}^\intercal = -\mathbf{L}, \mathbf{M}^\intercal = \mathbf{M}$.
    - Energy and Entropy function(al)s E, S .
- Want to capture $\dot{E} = 0, \dot{S} \geq 0$.
    - How to appropriately “stitch together” reversible and irreversible parts?

Metriplectic Systems

- Note,

$$\dot{E}(\mathbf{x}) = \dot{\mathbf{x}} \cdot \nabla E = \cancelto{0}{\mathbf{L}\nabla E \cdot \nabla E} + \mathbf{M}\nabla S \cdot \nabla E = \boxed{\nabla S \cdot \mathbf{M}\nabla E},$$

$$\dot{S}(\mathbf{x}) = \dot{\mathbf{x}} \cdot \nabla S = \mathbf{L}\nabla E \cdot \nabla S + \mathbf{M}\nabla S \cdot \nabla S = \boxed{-\nabla E \cdot \mathbf{L}\nabla S} + |\nabla S|^2_{\mathbf{M}}$$

- Solution? Prescribed degeneracies!
  - Choose $\mathbf{L}\nabla S = \mathbf{M}\nabla E = \mathbf{0}$.

Example: Thermoelastic Double Pendulum

$$\begin{pmatrix} \dot{\boldsymbol{q}}_1 \\ \dot{\boldsymbol{q}}_2 \\ \dot{\boldsymbol{p}}_1 \\ \dot{\boldsymbol{p}}_2 \\ \dot{S}_1 \\ \dot{S}_2 \end{pmatrix} = \begin{pmatrix} \boldsymbol{p}_1 \\ \boldsymbol{p}_2 \\ -\frac{\partial}{\partial \boldsymbol{q}_1}(E_1 + E_2) \\ -\frac{\partial}{\partial \boldsymbol{q}_2}(E_1 + E_2) \\ T_1^{-1} T_2 - 1 \\ T_1 T_2^{-1} - 1 \end{pmatrix}$$

- State variable

$$\mathbf{x} = \begin{pmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \mathbf{p}_1 & \mathbf{p}_2 & S_1 & S_2 \end{pmatrix}^\intercal$$

$$L = \begin{pmatrix} \mathbf{0}_{4\times 4} & \boldsymbol{S} \\ -\boldsymbol{S}^\top & \mathbf{0}_{6\times 6} \end{pmatrix}, \quad M = \begin{pmatrix} \mathbf{0}_{8\times 8} & \mathbf{0}_{8\times 2} \\ \mathbf{0}_{2\times 8} & \boldsymbol{T} \end{pmatrix}$$

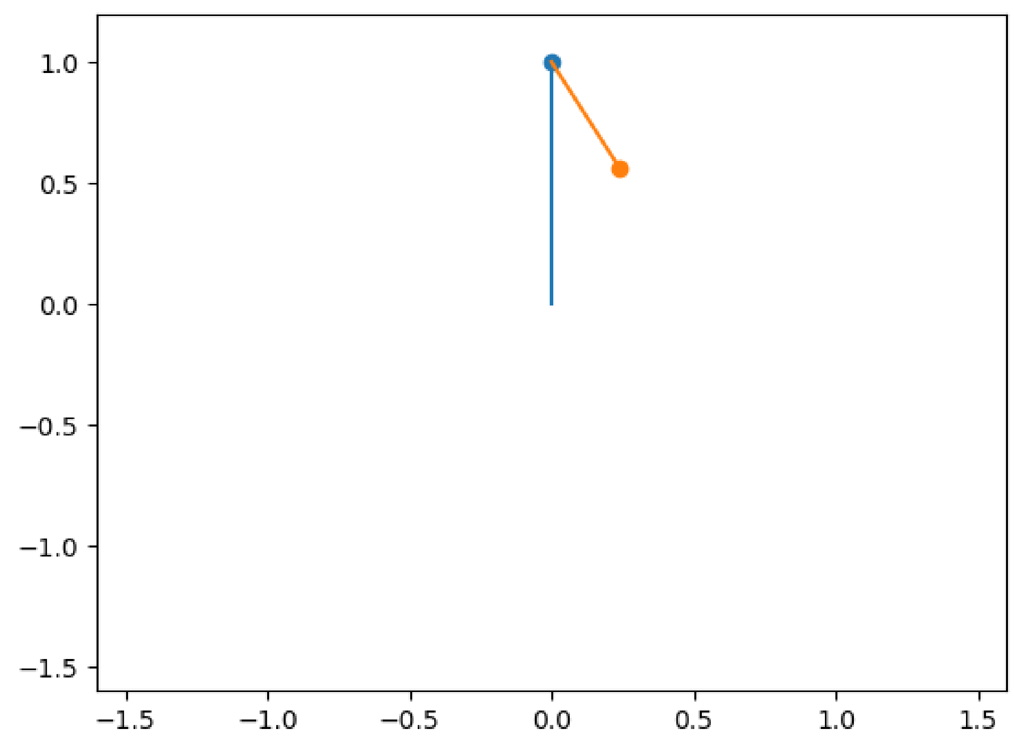
$$\boldsymbol{S} = \begin{pmatrix} \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} & \mathbf{0} \end{pmatrix}, \quad \boldsymbol{T} = \begin{pmatrix} \frac{T_2}{T_1} & -1 \\ -1 & \frac{T_1}{T_2} \end{pmatrix} \qquad T_i = \partial_{S_i} E_i$$

- Energy/Entropy: $S = S_1 + S_2$

$$E = \frac{1}{2}\left(|\mathbf{p}_1|^2 + |\mathbf{p}_2|^2\right) + E_1 + E_2$$

$$E_i = \frac{1}{2}(\log \lambda_i)^2 + \log \lambda_i + e^{S_i - \log \lambda_i} - 1$$

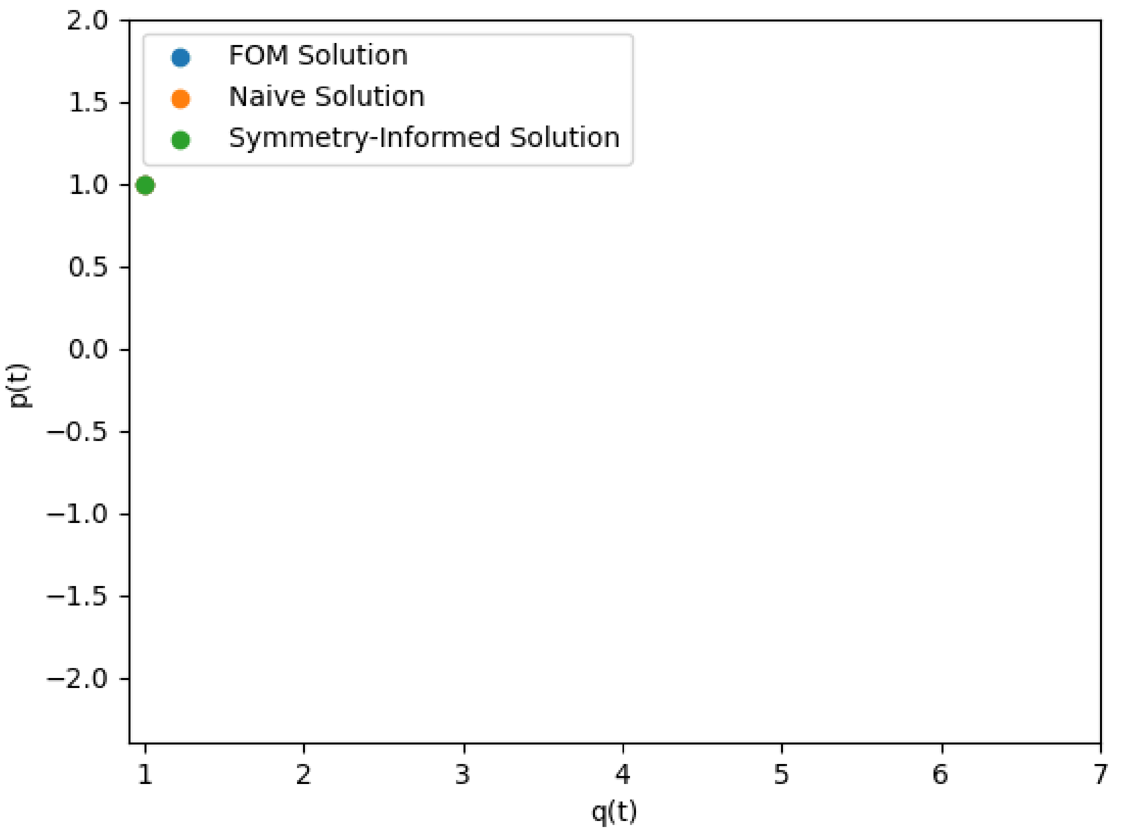
$$\lambda_1 = |\mathbf{q}_1|, \lambda_2 = |\mathbf{q}_2 - \mathbf{q}_1|$$

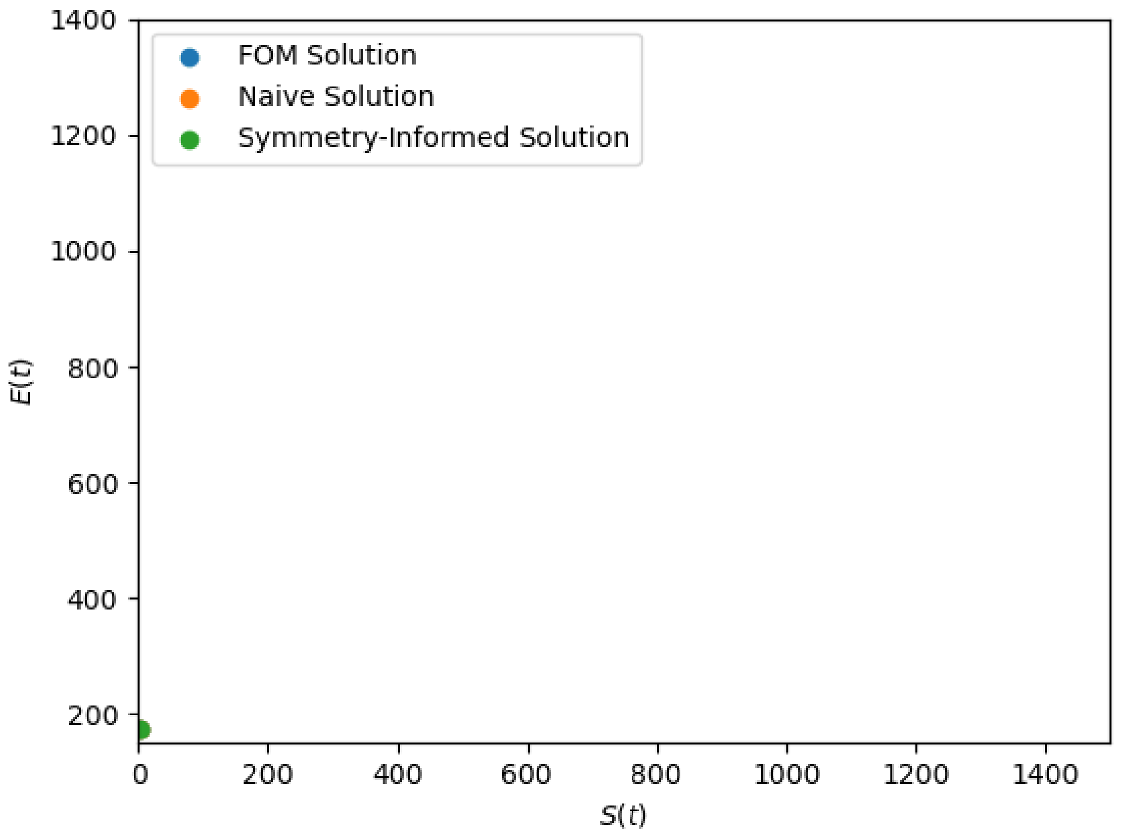


Metriplectic SP-ROM

- Want to reduce $\dot{\mathbf{x}} = \{\mathbf{x}, E\} + [\mathbf{x}, S] = \mathbf{L}\nabla E + \mathbf{M}\nabla S$.
  - $\hat{\mathbf{M}} = \mathbf{U}^\intercal\mathbf{M}\mathbf{U}$ and $\hat{\mathbf{L}} = \mathbf{U}^\intercal\mathbf{L}\mathbf{U}$ satisfy symmetries, but....
- Clearly $\hat{\mathbf{L}}\nabla\hat{S} = \mathbf{U}^\intercal\mathbf{L}\mathbf{U}\mathbf{U}^\intercal\nabla S \neq \mathbf{0}$ (same for $\hat{\mathbf{M}}\nabla\hat{E}$).
  - Metriplectic structure is not preserved!
  - No separation between reversible and irreversible parts.

Does this matter?





Metriplectic SP-ROM

- How to ensure $\hat{\mathbf{L}}\nabla\hat{S} = \hat{\mathbf{M}}\nabla\hat{E} = \mathbf{0}$.
    - Constrained optimization? Too expensive.
    - Penalty method? Too loose.
- Build in symmetries directly!
    - Can always parameterize at expense of increasing tensor degree.

Metriplectic SP-ROM

- If $\mathbf{L}\nabla S = \mathbf{0}$ and $\mathbf{L}^\intercal = -\mathbf{L}$, then $\boxed{\mathbf{L} = \boldsymbol{\xi}\left(\nabla S\right)}$.
  - $\boldsymbol{\xi}$ is order 3 totally antisymmetric tensor field $\xi^i_{jk}\,\boldsymbol{\partial}_i \otimes dx^j \otimes dx^k$.
- If $\mathbf{M}\nabla E = \mathbf{0}$ and $\mathbf{M}^\intercal = \mathbf{M}$, then $\boxed{\mathbf{M} = \boldsymbol{\zeta}\left(\nabla E, \nabla E\right)}$.
  - $\boldsymbol{\zeta}$ is rank 4 tensor field $\zeta^i_{kjl}\,\boldsymbol{\partial}_i \otimes dx^k \otimes dx^j \otimes dx^l$.
  - Satisfies $\zeta_{ikjl} = -\zeta_{kijl} = -\zeta_{iklj} = \zeta_{jlik}$.

Metriplectic SP-ROM

- Need to solve underdetermined systems!
  - For $\boldsymbol{L}$: $\xi^i_{jk}\partial^k S = L^i_j\,.$
  - For $\boldsymbol{M}$: $\zeta^i_{kjl}(\partial^k E)(\partial^l E) = M^i_j\;.$
- These are design decisions.

Why does this help?

- Galerkin projection $\tilde{\mathbf{x}} = \mathbf{U}\hat{\mathbf{x}}$ yields:

$$\dot{\hat{\mathbf{x}}} = \mathbf{U}^\intercal \xi\left(\nabla S\right)\nabla E + \mathbf{U}^\intercal \zeta\left(\nabla E, \nabla E\right)\nabla S$$

- If instead

$$\dot{\hat{\mathbf{x}}} = \overbrace{\boxed{\hat{\xi}\left(\nabla \hat{S}\right)}}^{\hat{\mathbf{L}}}\nabla \hat{E} + \overbrace{\boxed{\hat{\zeta}\left(\nabla \hat{E}, \nabla \hat{E}\right)}}^{\hat{\mathbf{M}}}\nabla \hat{S}$$

  - For some $\hat{\xi}, \hat{\zeta}$ with the right symmetries, then things will work!

Simplifying M

- Consider the eigenvalue decomposition $\mathbf{M} = \sum_{\alpha=1}^{r} \lambda_\alpha \, \mathbf{m}^\alpha \otimes \mathbf{m}^\alpha$.
  - Suppose $\mathbf{m}^\alpha = \mathbf{A}^\alpha \nabla E$ where $A^\alpha_{ij} = -A^\alpha_{ji}$.
- Can choose $\boxed{\zeta = \sum_{\alpha=1}^{r} \lambda_\alpha \, \mathbf{A}^\alpha \otimes \mathbf{A}^\alpha}$.
- Automatically preserves symmetries.
  - Requires solving $A^\alpha_{ij} \partial^j E = m^\alpha_i$ (design decision).

Metriplectic ROM

- All together: $\dot{\hat{\mathbf{x}}} = \hat{\mathbf{L}}\nabla\hat{E} + \hat{\mathbf{M}}\nabla\hat{S}$
$$= \hat{\boldsymbol{\xi}}\left(\nabla\hat{S}\right)\nabla\hat{E} + \hat{\zeta}\left(\nabla\hat{E},\nabla\hat{E}\right)\nabla\hat{S}$$
- **Theorem:** if $\mathbf{U}$ is a POD basis and $\boldsymbol{\xi}, \zeta, \nabla E, \nabla S$ are regular,

$$\int_{t=0}^{T} \|\mathbf{x}(t) - (\mathbf{x}_0 + \mathbf{U}\hat{\mathbf{x}}(t))\|^2 \leq \boxed{C\sum_{j>n}\sigma_j^2} \to 0$$

Recap: what's necessary?

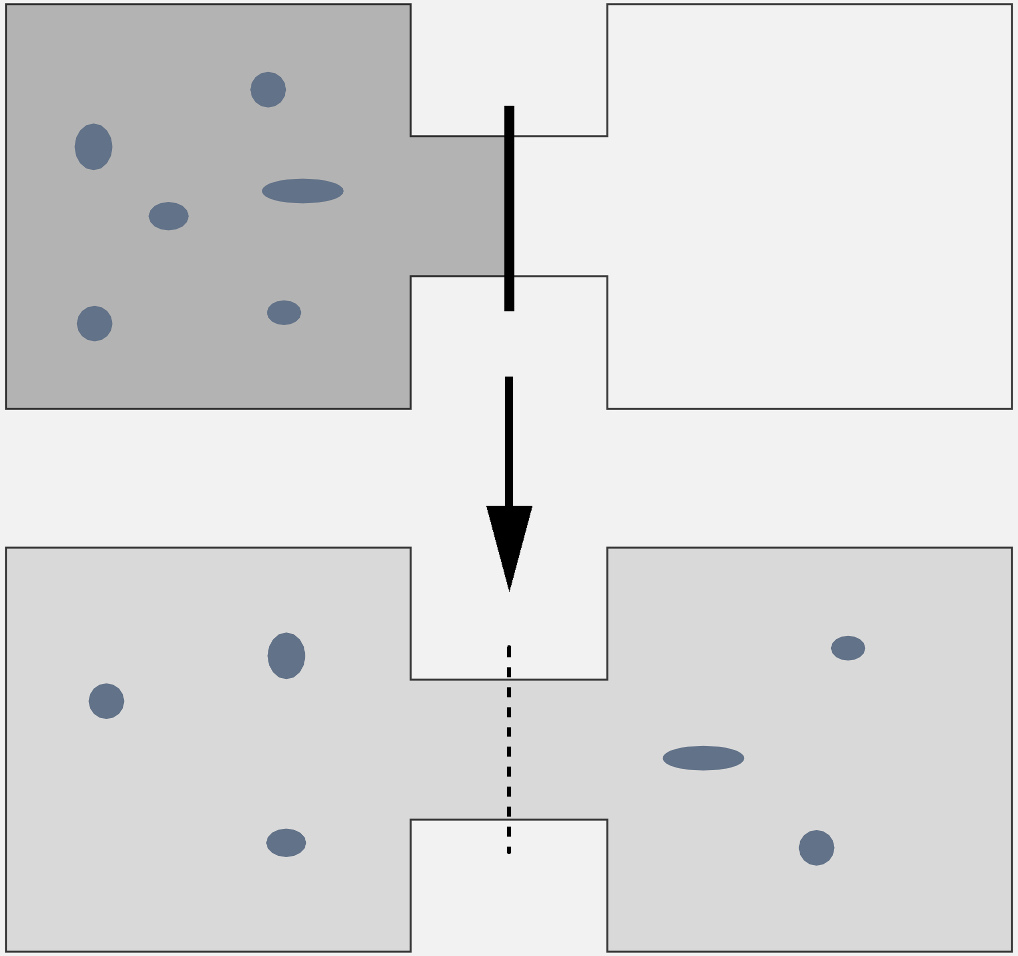
- Given: $\mathbf{L}, \mathbf{M}, \nabla E, \nabla S$ defining metriplectic system.
- Compute eigenvalue decomposition $\mathbf{M} = \sum_{\alpha=1}^{r} \lambda_\alpha \, \mathbf{m}^\alpha \otimes \mathbf{m}^\alpha$.
- Solve $\mathbf{L} = \boldsymbol{\xi}\left(\nabla S\right)$ and $\mathbf{m}^\alpha = \mathbf{A}^\alpha \nabla E$ (freedom here).
- Compute $\hat{\boldsymbol{\xi}} = \mathbf{U}^\intercal \boldsymbol{\xi}\left(\mathbf{U}\right)\mathbf{U}$ and $\hat{\mathbf{A}}^\alpha = \mathbf{U}^\intercal \mathbf{A}^\alpha \mathbf{U}$.
- *Assemble RO quantities: $\hat{\mathbf{L}} = \hat{\boldsymbol{\xi}}\left(\nabla \hat{S}\right)$, $\hat{\mathbf{M}} = \sum_{\alpha=1}^{r} \lambda_\alpha \, \hat{\mathbf{A}}^\alpha \nabla \hat{E} \otimes \hat{\mathbf{A}}^\alpha \nabla \hat{E}$.

Toy example: two gas containers

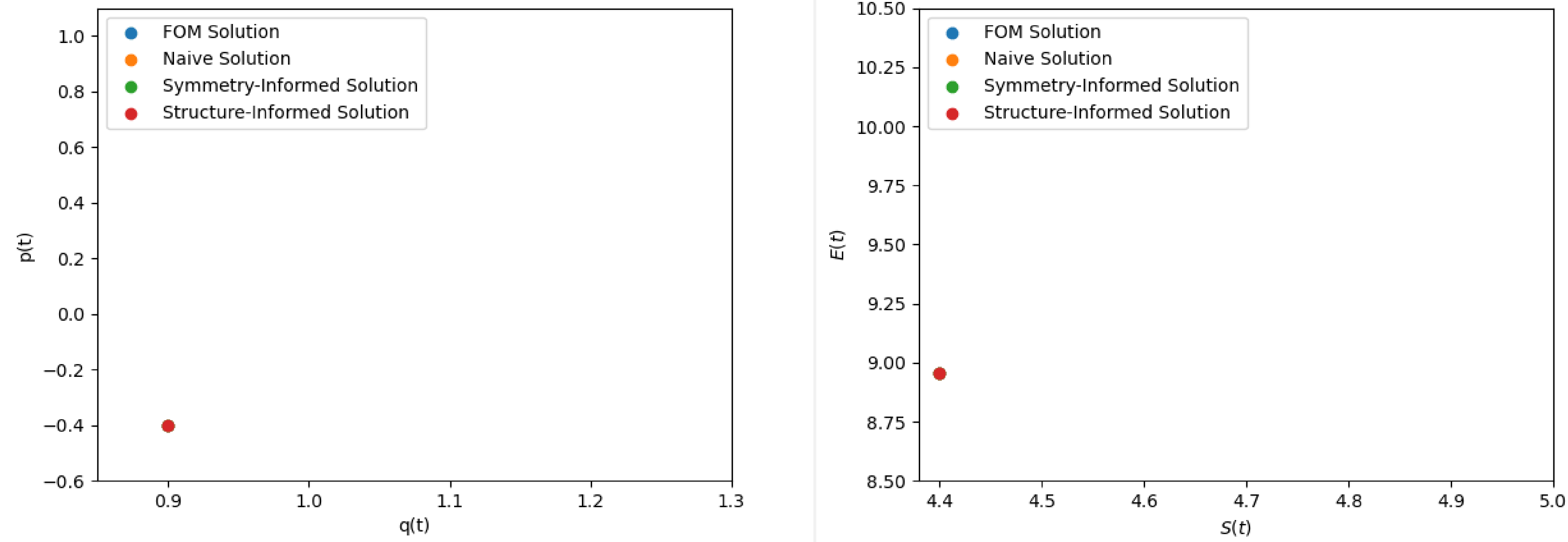
- Variables q, p, S_1, S_2 .
- Energy: $E(\mathbf{x}) = \frac{p^2}{2m} + \underbrace{\left(\frac{e^{\frac{S_1}{Nk_B}}}{\hat{c}q}\right)^{\frac{2}{3}}}_{E_1} + \underbrace{\left(\frac{e^{\frac{S_1}{Nk_B}}}{\hat{c}(2-q)}\right)^{\frac{2}{3}}}_{E_2}$.
- Entropy: $S(\mathbf{x}) = S_1 + S_2$.

$T_i = \partial_{S_i} E_i$

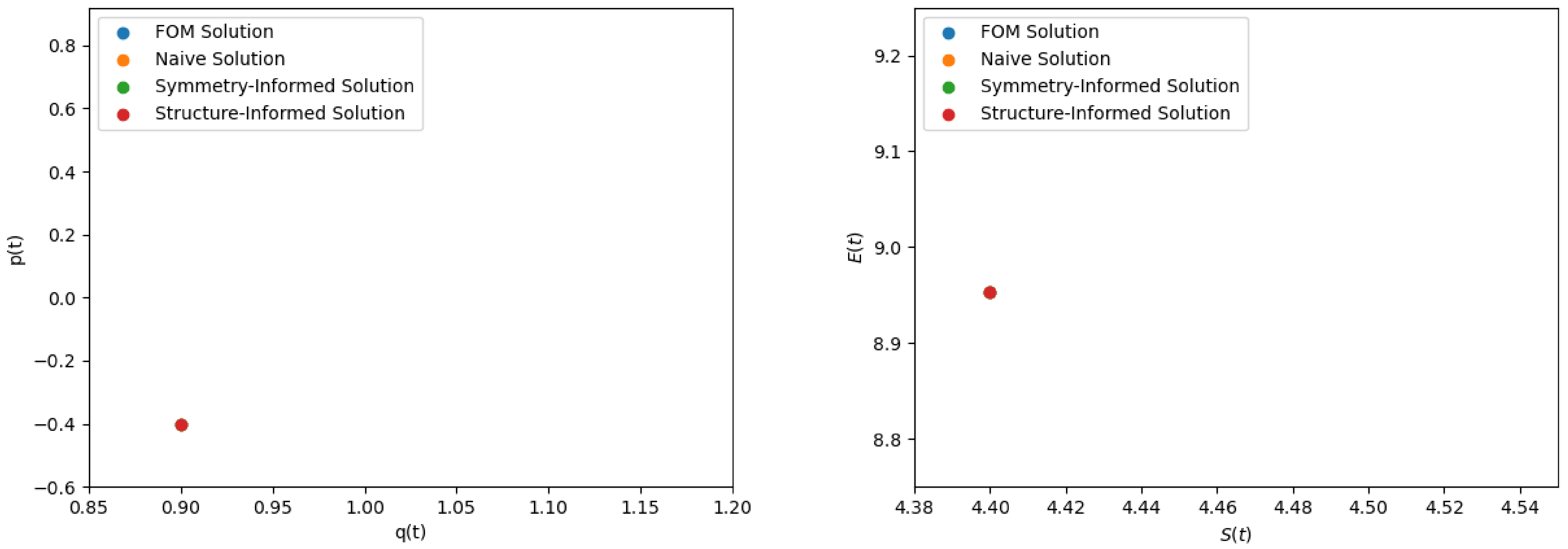
$$\mathbf{L} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \mathbf{M} = \gamma \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & T_1^{-2} & -(T_1T_2)^{-1} \\ 0 & 0 & -(T_1T_2)^{-1} & T_2^{-2} \end{pmatrix}$$



Results: two gas containers (3 modes)



Results: two gas containers (4 modes)



Is this enough?

- **Good:** Explicit recipe, exact structure preservation, convergence.
- **Bad:** Requires storage of two sparse degree 3 tensors.
  - $\boldsymbol{\xi}$ contains $\binom{N}{3} \ll N^3$ independent components.
  - $\mathbf{A}$ contains $r\binom{N}{2} \ll N^3$ independent components.
- Still too expensive. Any way to reduce cost?

Exterior algebra (EA)

- Recall the EA on V: $\Lambda(V) = T(V)/\{\mathbf{v} \otimes \mathbf{v} \,|\, \mathbf{v} \in V\}$
  - For example: $\mathbf{v} \wedge \mathbf{w} = \frac{1}{2}(\mathbf{v} \otimes \mathbf{w} - \mathbf{w} \otimes \mathbf{v})$ (DON'T store this)
- Advantage? Can multiply analytically first.
  - $\mathbf{v} \cdot (\mathbf{w}_1 \wedge \mathbf{w}_2 \wedge \ldots \wedge \mathbf{w}_n) = \sum_{i=1}^{n} (-1)^{i-1} (\mathbf{v} \cdot \mathbf{w}_i)\, \mathbf{w}_1 \wedge \ldots \wedge \widehat{\mathbf{w}_i} \wedge \ldots \wedge \mathbf{w}_n$
  - So, $\mathbf{v} \cdot (\mathbf{u} \wedge \mathbf{W}^k) = (\mathbf{v} \cdot \mathbf{u})\, \mathbf{W}^k - \mathbf{u} \wedge (\mathbf{v} \cdot \mathbf{W}^k)$.

Why is this useful?

- Identify L with the bivector sum $\mathbf{L} = \sum_{j<i} L^{ij}\, \mathbf{e}_i \wedge \mathbf{e}_j$.

- We have $\mathbf{L}\cdot\mathbf{v} = (-1)^{1(2+1)}\mathbf{v}\cdot\mathbf{L} = \boxed{\sum_{j<i} L^{ij} v_j \mathbf{e}_i - \sum_{j>i} L^{ji} v_j \mathbf{e}_i} = \mathbf{L}\mathbf{v}$.

  $L^{ii} = 0$

- So, define $\boldsymbol{\xi} = \mathbf{L} \wedge \mathbf{s}_{k_0}$.
  - Because of our design decision, $\mathbf{s}_{k_0} = \mathbf{e}_{k_0} / S^{k_0}$.

- $\boldsymbol{\xi}\left(\nabla S\right) = \left(\nabla S \cdot \mathbf{L}\right) \wedge \mathbf{s}_{k_0} + \underbrace{\boxed{\left(\mathbf{s}_{k_0} \cdot \nabla S\right)}}_{=1} \mathbf{L} = -\mathbf{L}\nabla S \wedge \mathbf{s}_{k_0} + \mathbf{L} = \mathbf{L},$

Why is this useful?

- Now, structure preservation is guaranteed by .

$$\hat{\mathbf{L}} = \hat{\boldsymbol{\xi}}\left(\nabla \hat{S}\right) = \left(\mathbf{U}^\intercal \mathbf{L} \mathbf{U} \wedge \mathbf{U}^\intercal \mathbf{s}_{k_0}\right) \cdot \nabla \hat{S} = \boxed{\bar{\mathbf{L}} \nabla \hat{S} \wedge \mathbf{s}_{k_0}} + \left(\hat{\mathbf{s}}_{k_0} \cdot \nabla \hat{S}\right) \bar{\mathbf{L}}$$

since

$$\hat{\mathbf{L}} \nabla \hat{S} = \boxed{(0)\hat{\mathbf{s}}_{k_0} + \left(\hat{\mathbf{s}}_{k_0} \cdot \nabla \hat{S}\right) \bar{\mathbf{L}} \nabla \hat{S}} - \left(\hat{\mathbf{s}}_{k_0} \cdot \nabla \hat{S}\right) \bar{\mathbf{L}} \nabla \hat{S} \quad .$$

- Only need to store $\bar{\mathbf{L}}$ and $\hat{\mathbf{s}}_{k_0} = \mathbf{U}^{k_0} / S^{k_0}$!!

Savings?

$$\mathbf{m}^\alpha \leftarrow \sqrt{\lambda_\alpha}\,\mathbf{m}^\alpha$$

- Similarly, choose $\mathbf{A}^\alpha = \mathbf{a}^\alpha_{k_1} \wedge \mathbf{e}_{k_1}$ where $\mathbf{a}_{k_1} = \boxed{\mathbf{m}^\alpha}/E^{k_1}$.
- Then, $\hat{\mathbf{A}}^\alpha = \hat{\mathbf{a}}^\alpha_{k_1} \wedge \mathbf{U}^{k_1}$ where $\hat{\mathbf{a}}^\alpha_{k_1} = \mathbf{U}^\intercal \mathbf{m}^\alpha / E^{k_1}$.
- Leads to $\hat{\mathbf{A}}^\alpha \nabla \hat{E} = \left(\nabla \hat{E} \cdot \mathbf{U}^{k_1}\right) \hat{\mathbf{a}}^\alpha_{k_1} - \left(\nabla \hat{E} \cdot \hat{\mathbf{a}}^\alpha_{k_1}\right) \mathbf{U}^{k_1}$
- No need to store SS matrices.

Savings?

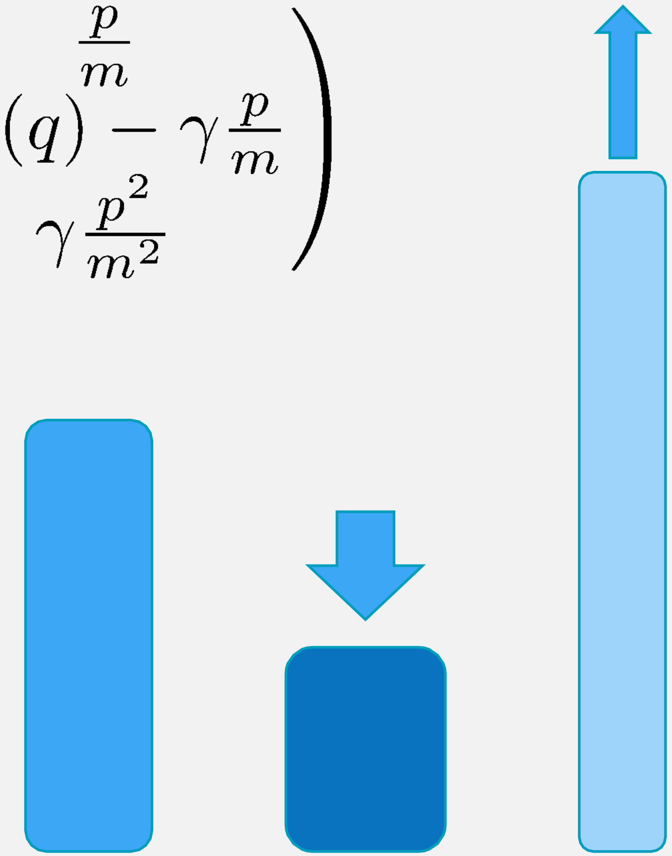
- We have $$\hat{\boldsymbol{\xi}} : \boxed{n^3} \rightarrow \boxed{n + \binom{n}{2}},$$ $$\hat{\mathbf{A}} : \boxed{rn^2} \rightarrow \boxed{n(r+1)}$$
- Makes metriplectic ROM feasible for larger problems.
  - *Make the algebra work for you!*

Example: Damped Thermoelastic Rod

- 1-D elastic rod with coordinate *s*.
  - damped Hamiltonian system with friction.

$$\begin{pmatrix} \dot{q} \\ \dot{p} \\ \dot{S} \end{pmatrix} = \begin{pmatrix} \frac{p}{m} \\ V'(q) - \gamma \frac{p}{m} \\ \gamma \frac{p^2}{m^2} \end{pmatrix}$$

$$\begin{aligned} E(p,q,e) &= H(p,q) + S(e) \\ &= \int_0^{\ell} \left(\frac{p(s)^2}{2m(s)} + V\left(q(s)\right) \right) + \int_0^{\ell} e(s) \end{aligned}$$



- V a given potential function.

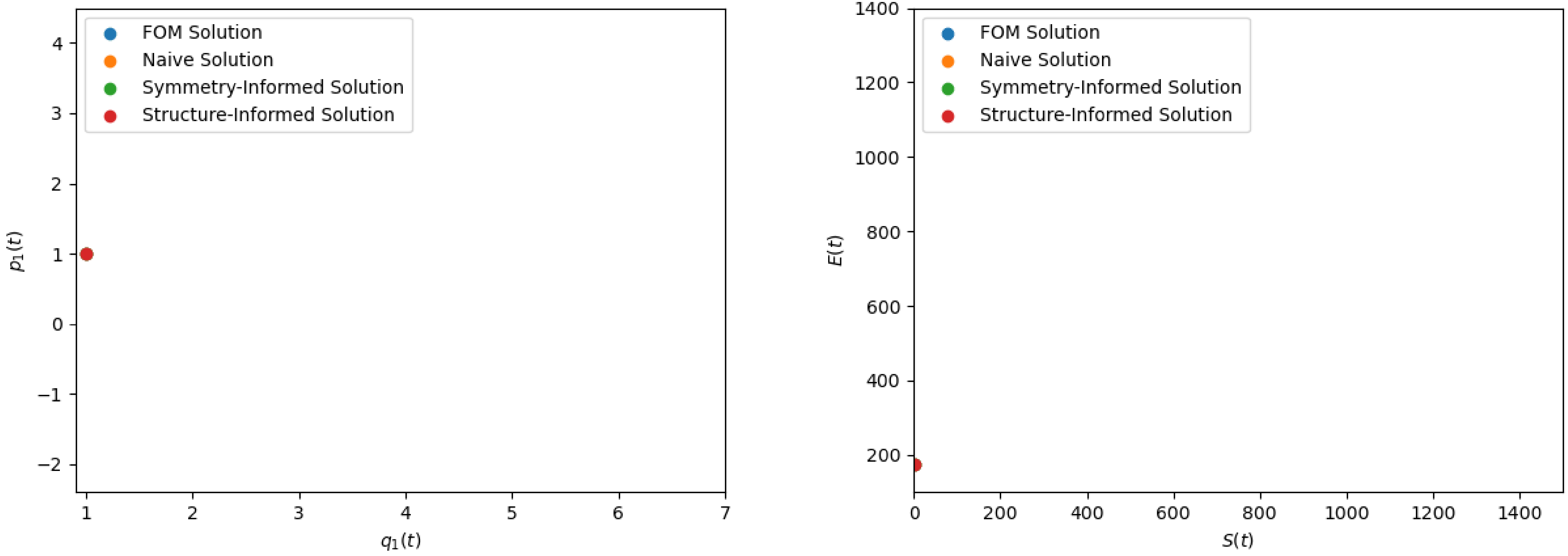
Example: Damped Thermoelastic Rod

- Discretization yields $\mathbf{x} = \begin{pmatrix}\mathbf{q} & \mathbf{p} & S\end{pmatrix}^\intercal \in \mathbb{R}^{2N+1}$. $\qquad \nabla S = \begin{pmatrix}\mathbf{0}\\ \mathbf{0}\\ 1\end{pmatrix}$

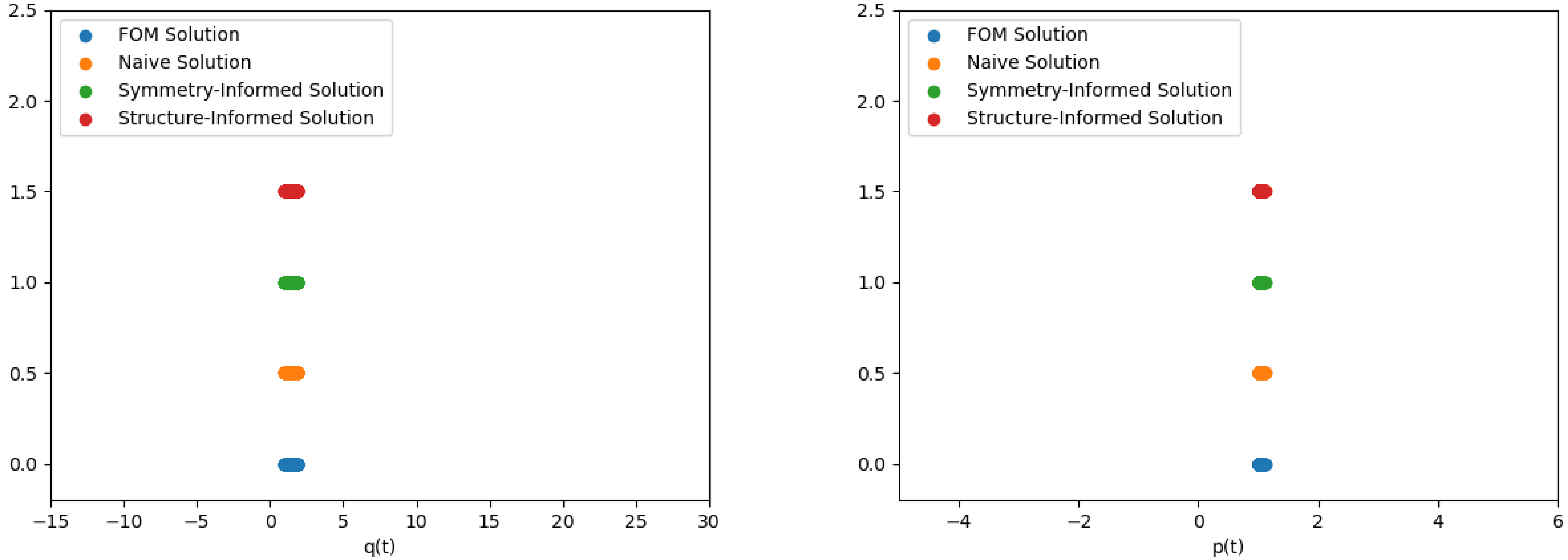
$$\mathbf{L} = \begin{pmatrix}\mathbf{0}_{N\times N} & \mathbf{I} & \mathbf{0}\\ -\mathbf{I} & \mathbf{0}_{N\times N} & \mathbf{0}\\ \mathbf{0} & \mathbf{0} & 0\end{pmatrix}, \quad \mathbf{M}(\mathbf{x}) = \gamma\begin{pmatrix}\mathbf{0}_{N\times N} & \mathbf{0}_{N\times N} & \mathbf{0}\\ \mathbf{0}_{N\times N} & \mathbf{I} & -\frac{\mathbf{p}}{m}\\ \mathbf{0} & -\frac{\mathbf{p}^\intercal}{m} & \left(\frac{|\mathbf{p}|}{m}\right)^2\end{pmatrix} \quad \nabla E(\mathbf{x}) = \begin{pmatrix}\mathbf{V}'(\mathbf{q})\\ \frac{\mathbf{p}}{m}\\ 1\end{pmatrix}$$

- Notice, $\mathbf{M} = \sum_{\alpha=1}^{N} \mathbf{m}^\alpha \otimes \mathbf{m}^\alpha, \qquad \mathbf{m}^\alpha = \sqrt{\gamma}\begin{pmatrix}\mathbf{0} & \mathbf{e}_\alpha & -\frac{p_\alpha}{m}\end{pmatrix}^\intercal,$
- Can choose $\hat{\boldsymbol{\xi}} = \bar{\mathbf{L}} \wedge \mathbf{U}^{2N+1}, \qquad \hat{\mathbf{A}}^\alpha(\tilde{\mathbf{x}}) = \mathbf{U}^\intercal \mathbf{m}^\alpha(\tilde{\mathbf{x}}) \wedge \mathbf{U}^{2N+1}$

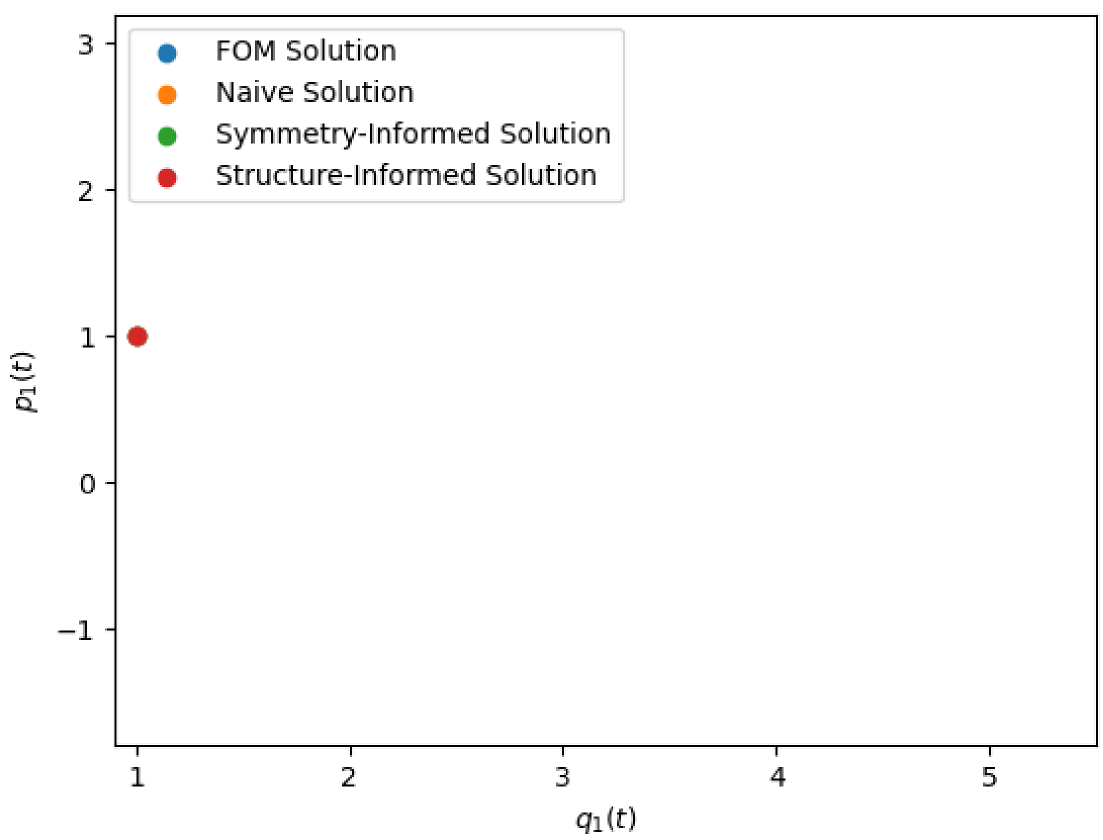
Results: Damped Thermoelastic Rod (10 modes)

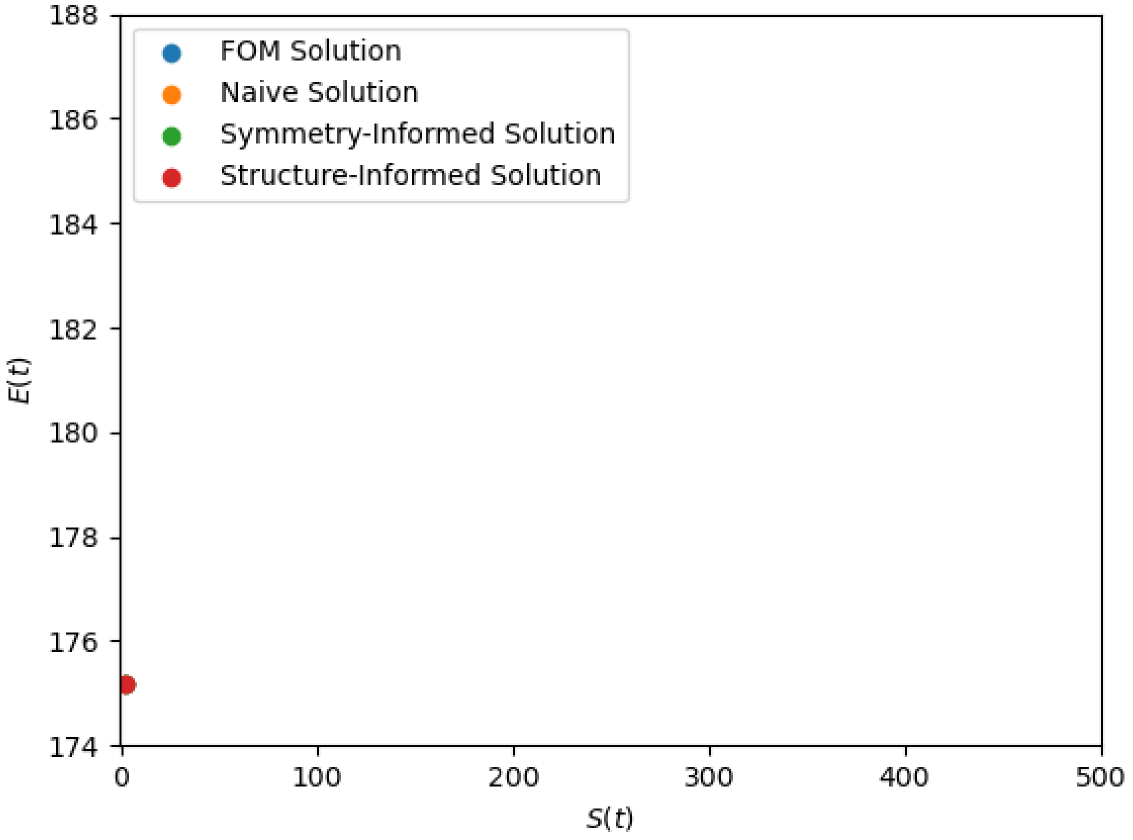


Results: Damped Thermoelastic Rod (10 modes)

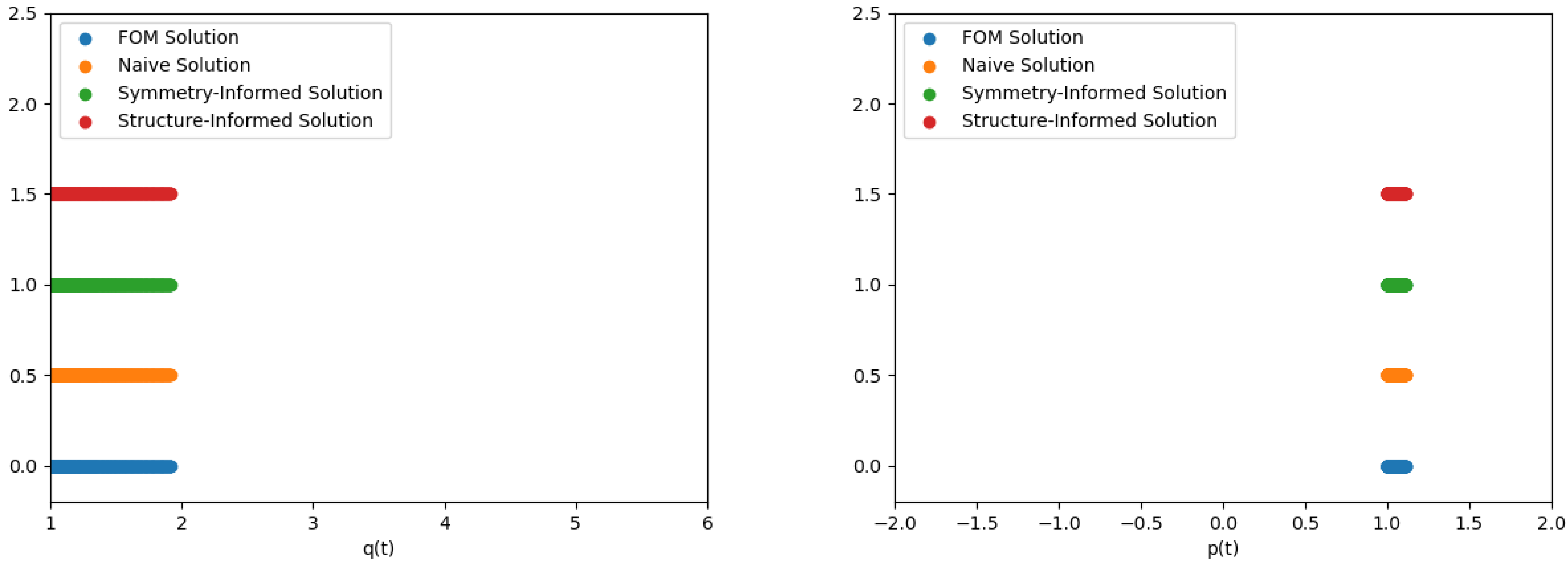


Results: Damped Thermoelastic Rod (60 modes)

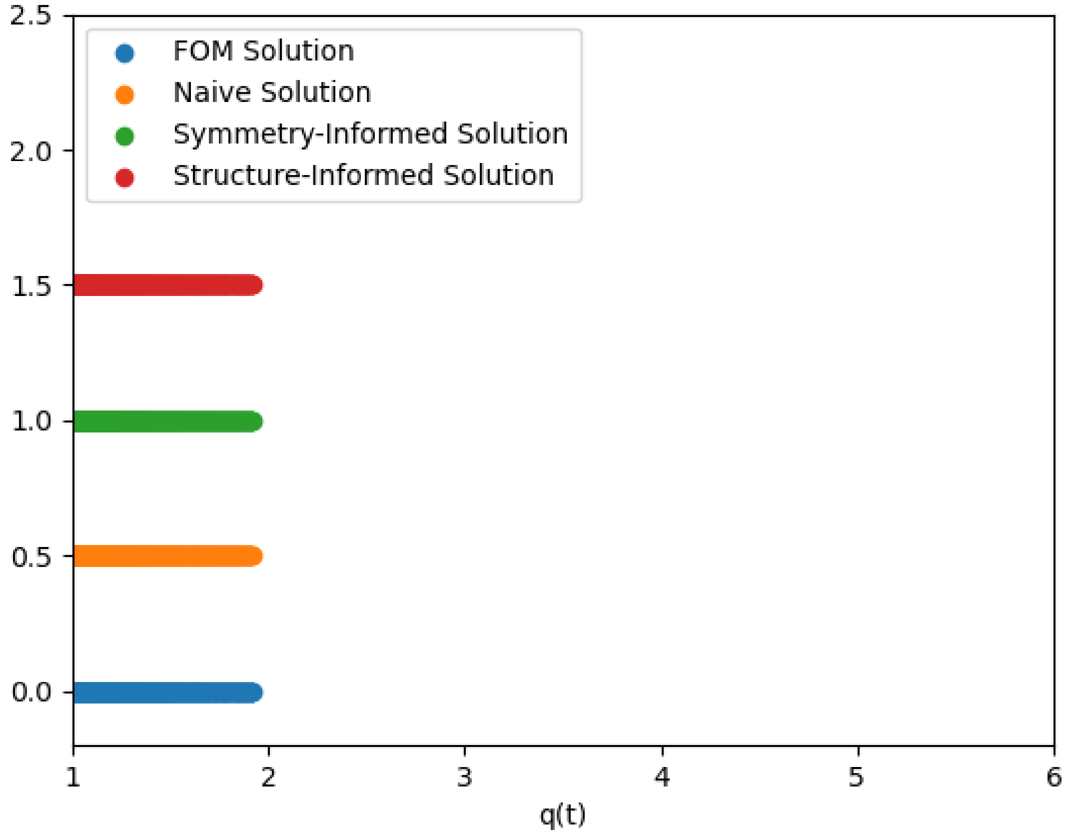


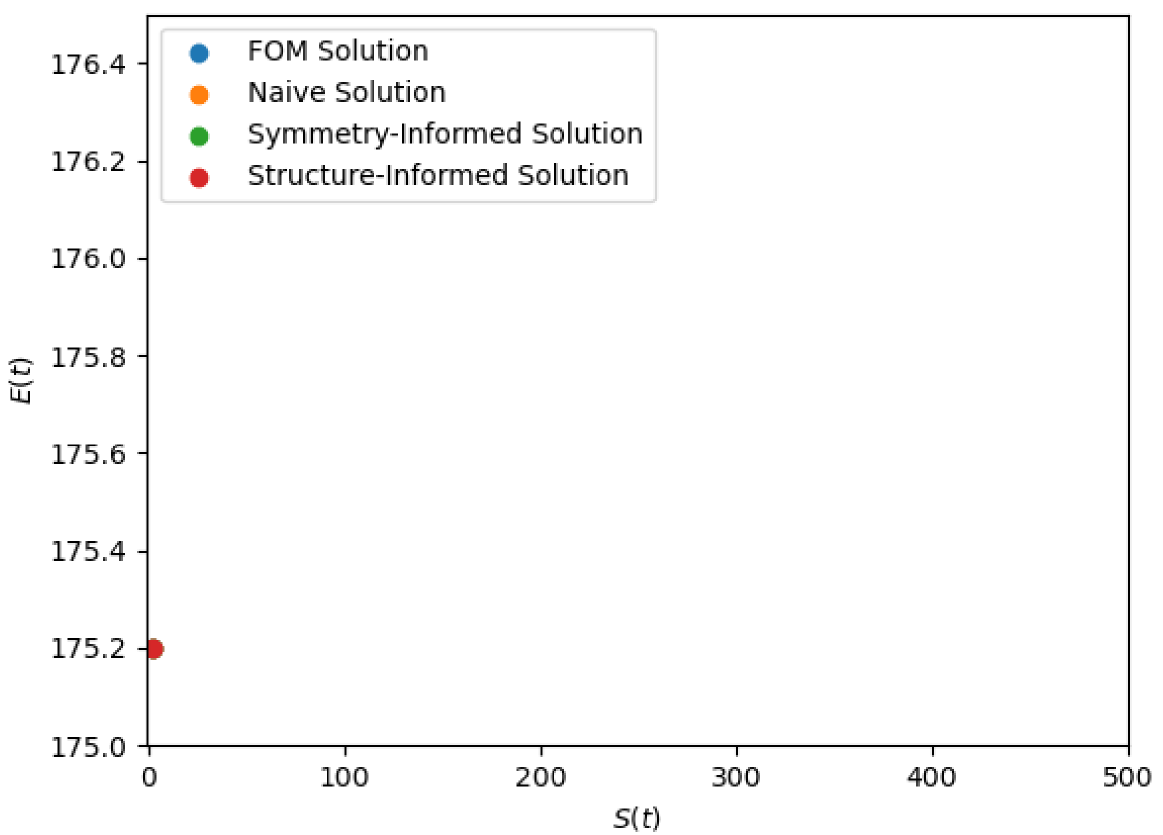


Results: Damped Thermoelastic Rod (60 modes)



Results: Damped Thermoelastic Rod (120 modes)





What's next?

- Structure-preserving hyper-reduction for nonlinearities.
  - Need non-intrusive version!!
- Good methods for Lagrangian systems.
  - Extension to Euler-Poincare, Lie-Poisson.

$$\frac{\partial f}{\partial t} = -\mathcal{J}^{ij} H_j f_i + \frac{1}{2} D \mathcal{J}^{ik} \frac{\partial}{\partial x^i}\left[f \mathcal{J}^{jk} \frac{\partial}{\partial x^j} \left(\log f + \beta H\right)\right],$$

$$\{F, G\} = \int_\Omega f \frac{\partial}{\partial x^i}\left(\frac{\delta F}{\delta f}\right)_\beta \mathcal{J}^{ij} \frac{\partial}{\partial x^j}\left(\frac{\delta G}{\delta f}\right)_\beta dV,$$

$$[F, G] = \frac{D}{2} \int_\Omega f \frac{\partial}{\partial x^i}\left(\frac{\delta F}{\delta f}\right)_\beta \mathcal{J}^{ik} \mathcal{J}^{jk} \frac{\partial}{\partial x^j}\left(\frac{\delta G}{\delta f}\right)_\beta dV,$$

Naoki Sato, Dissipative brackets for the Fokker–Planck equation in Hamiltonian systems and characterization of metriplectic manifolds, Physica D: Nonlinear Phenomena, Volume 411, 2020.

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, “Canonical and Noncanonical Hamiltonian Operator Inference”, (coming soon!)

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