Preserving Lagrangian Structure in Data-driven Reduced-order Modeling of Large-scale Dynamical Systems

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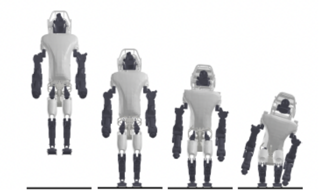
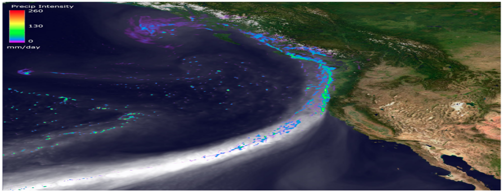
Structured Physical Systems are Everywhere!



(a) Dojo [Howell et al., 2022]



(b) Atmospheric river [Laurtizen et al., 2022]

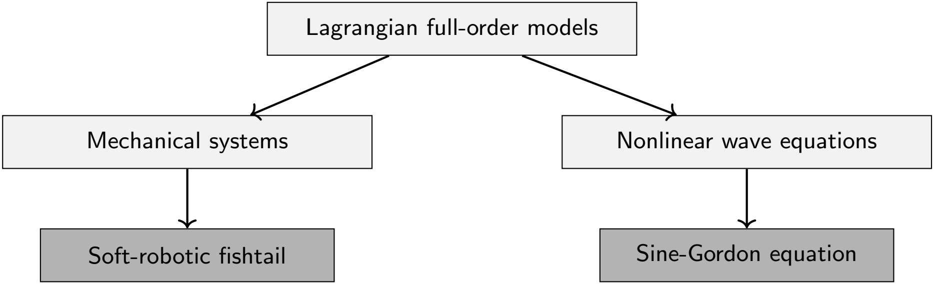
- Physical systems have interesting properties like conservation laws, symplecticity, reversibility or configuration space structure
- Structure-preserving methods preserve underlying geometric structure
  - Conserve discrete quantities which are close to continuous quantity
  - Reproduce long-time behavior
- Long-time numerical simulation of large-scale systems using structure-preserving methods is computationally prohibitive

Need for physics-preserving surrogate models

Problem Setting

- Lagrange-d'Alembert principle

$$\delta \mathfrak{B}(\mathbf{q}) = \delta \int_{t_0}^{t_K} L(\mathbf{q}, \dot{\mathbf{q}}) \, \mathrm{d}t + \int_{t_0}^{t_K} \mathbf{f}(\mathbf{q}, \dot{\mathbf{q}}, t) \cdot \delta \mathbf{q} \, \mathrm{d}t = 0$$



Mechanical Systems with Nonconservative Forcing

- Forced Euler-Lagrange equations

$$\frac{\partial L(\mathbf{q}, \dot{\mathbf{q}})}{\partial \mathbf{q}} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L(\mathbf{q}, \dot{\mathbf{q}})}{\partial \dot{\mathbf{q}}}\right) + \mathbf{f}(\mathbf{q}, \dot{\mathbf{q}}, t) = \mathbf{0}$$

- Full-order model (FOM) governing equations

$$\boxed{\mathbf{M}\ddot{\mathbf{q}}(t) + \mathbf{C}\dot{\mathbf{q}}(t) + \mathbf{K}\mathbf{q}(t) = \mathbf{B}\mathbf{u}(t)}$$

  along with the output equation

$$\mathbf{y}(t) = \mathbf{E}\mathbf{q}(t)$$

- Key features
  1. Lagrangian symplectic structure
  2. Symmetric positive-definite property of system matrices
  3. Energy conservation for conservative mechanical systems

Goal: Learning Lagrangian reduced-order models (ROMs) nonintrusively from data without assuming access to FOM operators

Related Work

1. Intrusive structure-preserving model reduction for Lagrangian systems ([Lall et al., 2004], [Carlberg et al., 2015])
   Drawback: Requires access to FOM operators

2. Structure-preserving neural networks ([Cranmer et al., 2019], [Lutter et al., 2019], [Gupta et al., 2020])
   Drawback: Ill-suited for high-dimensional systems

3. Nonintrusive model reduction via operator inference (OpInf)
   - Operator inference for nonlinear systems ([Peherstorfer and Willcox, 2016], [Benner et al., 2020])
   - Lift & Learn ([Qian et al., 2020], [Swischuk et al., 2020])

   Drawback: Does not preserve the Lagrangian structure

Key idea: Embed Lagrangian structure into OpInf framework

Problem Formulation: FOM Data

Given: Snapshot data matrices from Lagrangian FOM simulations

$$\mathbf{Q} = [\mathbf{q}_1, \cdots, \mathbf{q}_K] \in \mathbb{R}^{n \times K}$$

- Output snapshot matrix

$$\mathbf{Y} = [\mathbf{y}_1, \cdots, \mathbf{y}_K] \in \mathbb{R}^{p \times K}$$

- Input snapshot matrix

$$\mathbf{U} = [\mathbf{u}(t_1), \cdots, \mathbf{u}(t_K)] \in \mathbb{R}^{m \times K}$$

Next step: Project FOM data onto low-dimensional subspaces

Problem Formulation: Projection

- Computing POD basis via SVD

$$\mathbf{Q} = \mathbf{V}\Xi\mathbf{W}^\top$$

where $\mathbf{V} \in \mathbb{R}^{n\times n}$, $\Xi \in \mathbb{R}^{n\times n}$, and $\mathbf{W} \in \mathbb{R}^{K\times n}$

- Projecting FOM data to obtain reduced snapshot data

$$\hat{\mathbf{Q}} = \mathbf{V}_r^\top\mathbf{Q} = [\hat{\mathbf{q}}_1, \cdots, \hat{\mathbf{q}}_K] \in \mathbb{R}^{r\times K}$$

- Reduced time-derivative data

$$\dot{\hat{\mathbf{Q}}} = [\dot{\hat{\mathbf{q}}}_1, \cdots, \dot{\hat{\mathbf{q}}}_K] \in \mathbb{R}^{r\times K}, \qquad \ddot{\hat{\mathbf{Q}}} = [\ddot{\hat{\mathbf{q}}}_1, \cdots, \ddot{\hat{\mathbf{q}}}_K] \in \mathbb{R}^{r\times K}$$

Next step: Fit reduced operators to the projected trajectories in a structure-preserving way

Problem Formulation: Model Form for Learning ROM

- Reduced Lagrangian with reduced mass matrix $\hat{\mathbf{M}} = \mathbb{I}_r$

$$\hat{L}_r(\hat{\mathbf{q}}, \dot{\hat{\mathbf{q}}}) = \frac{1}{2}\dot{\hat{\mathbf{q}}}^\top \dot{\hat{\mathbf{q}}} - \frac{1}{2}\hat{\mathbf{q}}^\top \hat{\mathbf{K}}\hat{\mathbf{q}},$$

- Reduced forcing

$$\hat{\mathbf{f}}(\hat{\mathbf{q}}, \dot{\hat{\mathbf{q}}}, t) = \hat{\mathbf{C}}\dot{\hat{\mathbf{q}}} - \hat{\mathbf{B}}\mathbf{u}(t)$$

- Model form for learning Lagrangian ROMs based on $\hat{L}_r(\hat{\mathbf{q}}, \dot{\hat{\mathbf{q}}})$

$$\ddot{\hat{\mathbf{q}}}(t) + \hat{\mathbf{C}}\dot{\hat{\mathbf{q}}}(t) + \hat{\mathbf{K}}\hat{\mathbf{q}}(t) = \hat{\mathbf{B}}\mathbf{u}(t)$$

along with the reduced output equation

$$\mathbf{y}(t) = \hat{\mathbf{E}}\hat{\mathbf{q}}(t)$$

Model form ensures that the reduced models are Lagrangian

Novel Operator Inference for Mechanical Systems

- Constrained optimization problem to compute $\hat{\mathbf{C}} \in \mathbb{R}^{r \times r}, \hat{\mathbf{K}} \in \mathbb{R}^{r \times r}$, and $\hat{\mathbf{B}} \in \mathbb{R}^{r \times m}$

$$\min_{\substack{\hat{\mathbf{K}}=\hat{\mathbf{K}}^\top \succ 0, \hat{\mathbf{C}}=\hat{\mathbf{C}}^\top \succ 0, \\ \hat{\mathbf{B}}}} ||\ddot{\hat{\mathbf{Q}}} + \hat{\mathbf{C}}\dot{\hat{\mathbf{Q}}} + \hat{\mathbf{K}}\hat{\mathbf{Q}} - \hat{\mathbf{B}}\mathbf{U}||_F$$

  where the specific choice of $\hat{\mathbf{M}}$ simplifies the constrained inference problem ([Gosea, Gugercin, and Werner, 2023])
- Separate linear least-squares problem to compute $\hat{\mathbf{E}} \in \mathbb{R}^{p \times r}$

$$\min_{\hat{\mathbf{E}}} ||\mathbf{Y} - \hat{\mathbf{E}}\hat{\mathbf{Q}}||_F$$

- Constrained optimization problem solved using the semidefinite programming mode in CVX[1]

Structure-preserving learning of ROMs via hard constraints

[1] M. Grant and S. Boyd, CVX: Matlab software for disciplined convex programming, version 2.1, 2014

Novel Operator Inference for Nonlinear Wave Equations

$$\mathcal{L}(x, q, q_x, q_t) = \frac{1}{2}\left(\left(\frac{\partial q}{\partial t}\right)^2 - \left(\frac{\partial q}{\partial x}\right)^2\right) - U_{\text{nl}}(q)$$

- Use knowledge about the nonlinear potential energy U_{nl} at the PDE level to build the nonlinear forcing snapshot data matrix

$$\mathbf{F}_{\text{nl}} = [\mathbf{f}_{\text{nl}}(\mathbf{q}_1), \cdots, \mathbf{f}_{\text{nl}}(\mathbf{q}_K)] \in \mathbb{R}^{n \times K}$$

- Projecting FOM snapshot data $\mathbf{Q}$ and forcing snapshot data $\mathbf{F}_{\text{nl}}$

$$\hat{\mathbf{Q}} = \mathbf{V}_r^\top \mathbf{Q} \in \mathbb{R}^{r \times K}, \qquad \hat{\mathbf{F}}_{\text{nl}} = \mathbf{V}_r^\top \mathbf{F}_{\text{nl}} \in \mathbb{R}^{r \times K}$$

- Constrained optimization problem to compute $\hat{\mathbf{K}} \in \mathbb{R}^{r \times r}$

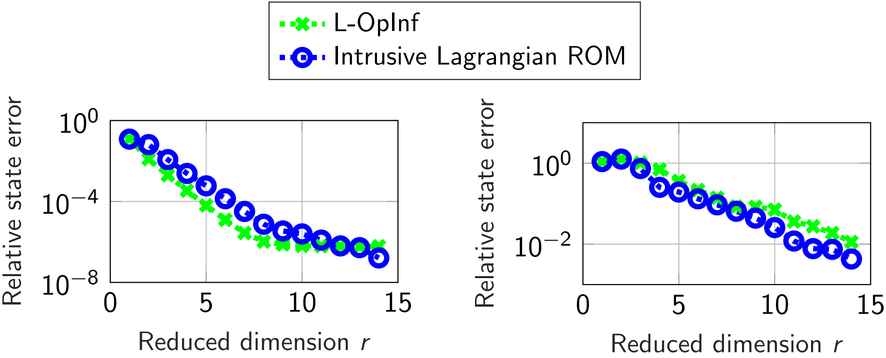
$$\min_{\hat{\mathbf{K}} = \hat{\mathbf{K}}^\top} \|\ddot{\hat{\mathbf{Q}}} - \hat{\mathbf{F}}_{\text{nl}} - \hat{\mathbf{K}}\hat{\mathbf{Q}}\|_F$$

Learned ROM operator $\hat{\mathbf{K}}$ respects the symmetric property introduced during the structure-preserving spatial discretization

Sine-Gordon Equation (n=2000): State Error

Nonlinear hyperbolic PDE with a nonpolynomial nonlinearity

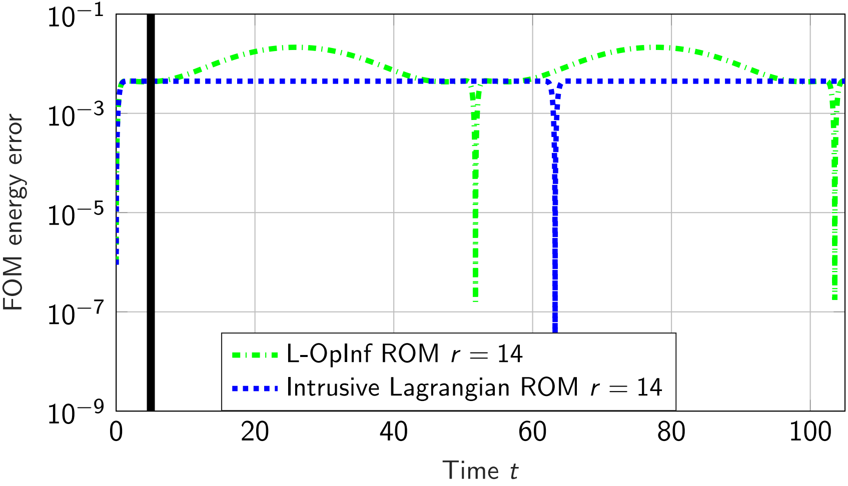
$$\frac{\partial^2 q}{\partial t^2} = \frac{\partial^2 q}{\partial x^2} - \sin(q)$$



(a) Training regime $[0, 5]$ s

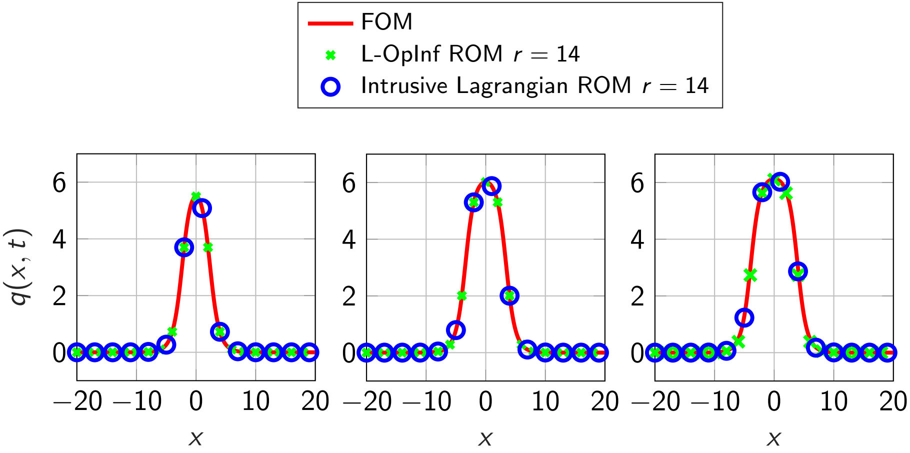
(b) Testing regime $[5, 25]$ s

Sine-Gordon Equation ($n = 2000$): Bounded Energy Error



Preserving Lagrangian structure yields stable ROMs with bounded energy error far outside the training data regime

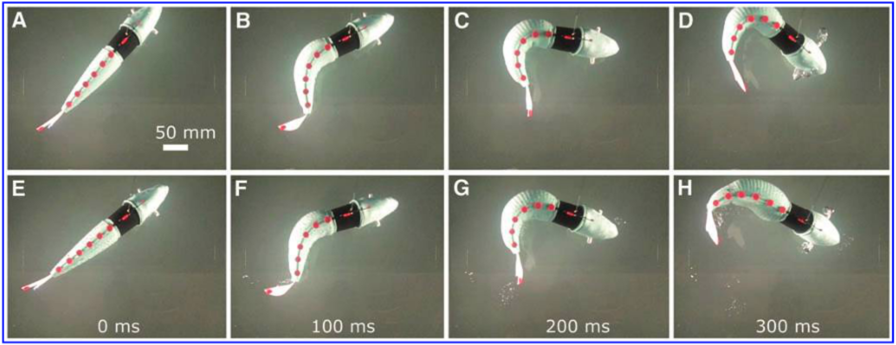
Sine-Gordon Equation ($n = 2000$): Extrapolation in Time



(a) $t = 5$ (b) $t = 15$ (c) $t = 25$

Accurate predictions 400% outside training time interval

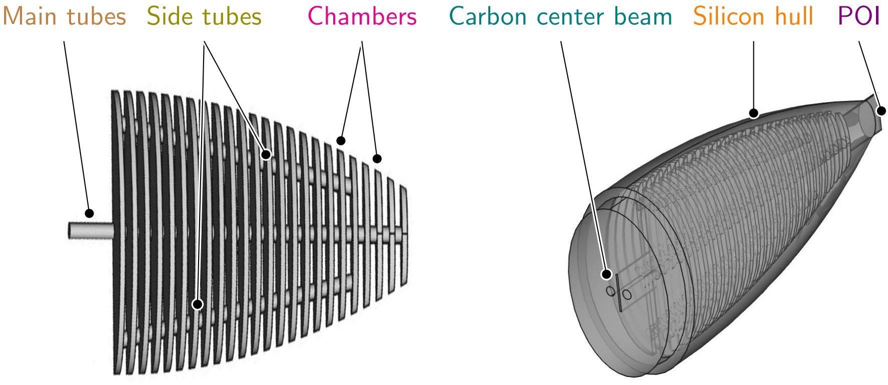
Soft-robotic Fishtail



- Soft robotic fish[2] designed to emulate escape responses in addition to forward swimming because such maneuvers require rapid body accelerations and continuum-body motion
- Fish's soft body is an array of fluidic elastomer actuators

[2] A. D. Marchese, C. D. Onal, and D. Rus, Autonomous soft robotic fish capable of escape maneuvers using fluidic elastomer actuators, Soft Robotics, 1 (2014), pp. 75–87.

Fishtail CAD Model[3]



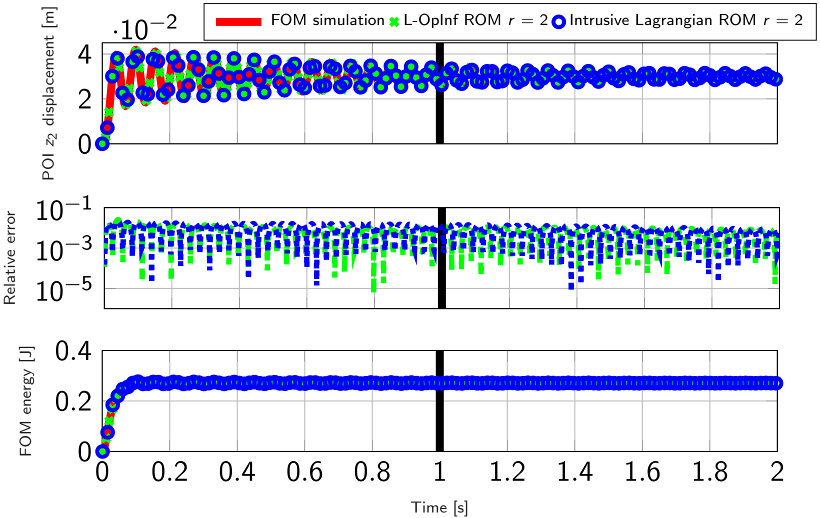
(a) Fluid chamber system

(b) Complete fishtail model

$$\rho \frac{\partial^2 \underline{q}(t, \mathbf{z})}{\partial t^2} = \nabla_{\mathbf{z}} \cdot \underline{\sigma}(t, \mathbf{z})$$

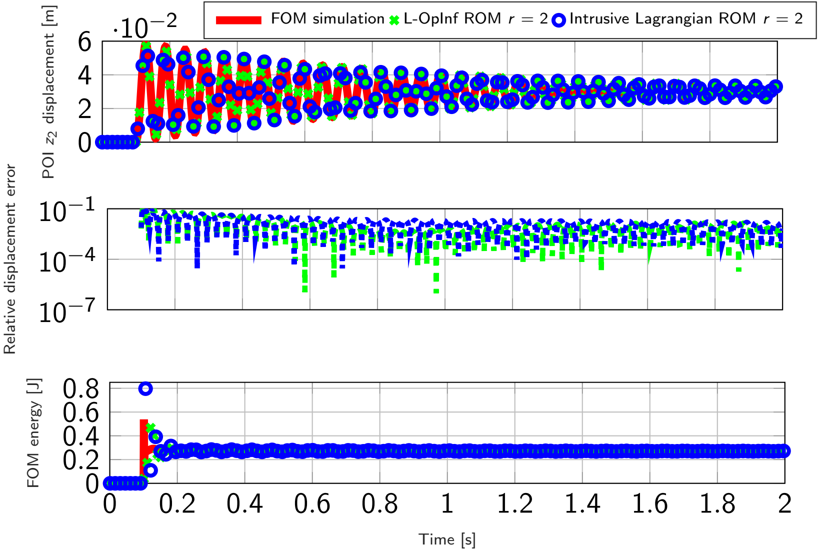
[3] D. Siebelts, A. Kater, and T. Meurer, Modeling and motion planning for an artificial fishtail, IFAC-PapersOnLine, 51 (2018), pp. 319–324.

Soft-robotic Fishtail ($n = 779,232$): Sigmoid Input



L-OpInf provides accurate predictions for forced mechanical systems

Soft-robotic Fishtail ($n = 779,232$): Step Input



L-OpInf works well even for unknown control inputs

Conclusions and Ongoing Work

- Lagrangian operator inference:
  - ensures reduced models are Lagrangian systems
  - respects the structure of system matrices
- Numerical results
  - Accurate long-time predictions far outside the training data regime
  - Robust to unknown control inputs
  - Stable ROMs with bounded FOM energy error
- Discussion about open research directions
  1. How to tackle unknown nonlinear terms?
  2. Theoretical results about stability and bounds on the FOM energy error
  3. Using lifting transformations in a structure-preserving way
- Ongoing work
  1. Combination with structure-preserving machine learning techniques to learn nonlinear potential energy terms from data
  2. Using data-driven quadratic manifold approximations for structure-preserving model reduction of transport-dominated problems

Thank you!

- **Preserving Lagrangian structure in data-driven reduced-order modeling of large-scale mechanical systems**
  Sharma, H., Kramer, B., arXiv:2203.06361
- **Symplectic model reduction of Hamiltonian systems using data-driven quadratic manifolds**
  Sharma, H., Mu, H., Buchfink, P., Geelen, R., Glas, S., Kramer, B., arXiv:2305.15490
- **Hamiltonian operator inference: Physics-preserving learning of reduced-order models for canonical Hamiltonian systems**
  Sharma, H., Wang, Z., Kramer, B., Physica D: Nonlinear Phenomena, Volume 431, 2022, 13312
- **Bayesian Identification of Nonseparable Hamiltonian Systems Using Stochastic Dynamic Models**
  Sharma, H., Galioto, N., Gorodetsky, A., Kramer, B., 2022 61st IEEE Conference on Decision and Control (CDC)