Structure-preserving Lift & Learn: Scientific machine learning for nonlinear conservative PDEs

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Workshop II: Learning Models from Data for Multi-Fidelity Fusion Plasma Physics
IPAM Long Program on Multi-Fidelity Methods for Fusion Energy
April 13 - 17, 2026

UC San Diego
JACOBS SCHOOL OF ENGINEERING
Mechanical and Aerospace Engineering

Thanks to my collaborators!

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(d) Gleb Pogudin (École Polytechnique)

Thanks to our sponsors:

- NSF: *CAREER: Goal-oriented Variable Transformations for Efficient Reduced-order and Data-driven Modeling* (2022-2027)
- ONR: *Nonlinear Data-driven and Structure-Preserving Hamiltonian Model Reduction* (2022-2025)
- DoD: *Geometric Structure-Preserving Model Reduction for Large-Scale Interconnected Systems* (2020).

Variable transformations and Quadratization

Learning dynamical systems

Given a simulator of a transient complex (e.g., plasma) process, i.e., given n-dim. data

$$\dot{\mathbf{Y}} = [\dot{\mathbf{y}}(t_0), \dot{\mathbf{y}}(t_0), \ldots, \dot{\mathbf{y}}(t_N)] \quad \text{and} \quad \mathbf{Y} = [\mathbf{y}(t_0), \mathbf{y}(t_0), \ldots, \mathbf{y}(t_N)]$$

If we are interested in learning the underlying dynamics[1], would we rather

1) Learn a general nonlinear approximation

$$\dot{\mathbf{y}}(t) = \mathbf{f}(\mathbf{y}(t)) \quad \Rightarrow \quad \min_{\theta} \|\dot{\mathbf{Y}} - \mathbf{f}_{\theta}(\mathbf{Y})\| \quad \text{e.g., ML, symbolic regression,...}$$

2) Learn a quadratic-linear polynomial form

$$\dot{\mathbf{y}}(t) = \mathbf{A}\mathbf{y}(t) + \mathbf{H}\mathbf{y}^2(t) \quad \Rightarrow \quad \min_{\mathbf{A}\in\mathbb{R}^{n\times n}, \mathbf{H}\in\mathbb{R}^{n\times n^2}} \|\dot{\mathbf{Y}} - \mathbf{H}\mathbf{Y}^2 - \mathbf{A}\mathbf{Y}\| \quad \Rightarrow \text{LS regression}$$

[1] ignoring issue of high dimensionality on this slide; as well as technicalities of min problems

What if we could quadratize dynamical systems?

ODE quadratization:

$$\dot{\mathbf{y}}(t) = \mathbf{f}(\mathbf{y}(t)) \qquad \xrightarrow{\bar{\mathbf{y}}=\tau_{\text{lift}}(\mathbf{y})} \qquad \dot{\bar{\mathbf{y}}}(t) = \mathbf{A}\mathbf{y}(t) + \mathbf{H}\mathbf{y}^2(t),$$

PDE quadratization:

$$\frac{\partial y(\mathbf{x},t)}{\partial t} = f(y(\mathbf{x},t)) \qquad \xrightarrow{\bar{y}=\tau_{\text{lift}}(y)} \qquad \frac{\partial \bar{y}(\mathbf{x},t)}{\partial t} = \mathcal{A}(\bar{y}(\mathbf{x},t)) + \mathcal{H}(\bar{y}(\mathbf{x},t)),$$

where $\mathcal{A}$ is a linear operator and $\mathcal{H}$ is a quadratic operator in $\mathbf{y}$.

Key observation: models are not unique!

The same evolutionary process can be modeled with different variables $\Rightarrow$ can improve computational modeling and analysis.

Example quadratization

Consider the cubic scalar PDE

$$y_t = y_x y^2.$$

Here we have one spatial derivative, so $h = 1$, and one polynomial $p_1(y, y_x) = y^2 y_x$. We introduce one ($\ell = 1$) new variable

$$w = q_1(y) = y^2,$$

which has no spatial derivative, so $s = 0$. With this new variable, the original PDE can be written as

$$\begin{cases} \underline{\partial_t y} = y^2 y_x = \underline{w y_x}, \\ \underline{\partial_t w} = 2 y y_t = 2 y^3 \partial_x y = \underline{w w_x}. \end{cases}$$

Thus, we have $H = 1$ and the quadratic monomials $h_1(y_x, w) = w y_x$, and $h_2(w, w_x) = w w_x$.

Exploiting quadratization in the literature

- Convexifying **optimization** problems via variable transformations [McCormick, 1976]
- **Analog computing** with chemical reaction networks requires quadratic forms; helps establish Turing completeness of elementary chemical reactions [Bournez et al., 2007, Fages et al., 2017, Hemery et al., 2020].
- Quadratized models appealing for **intrusive model reduction**, e.g., [Gu, 2011, Benner and Breiten, 2015, Benner et al., 2018, Kramer and Willcox, 2019, Kramer and Willcox, 2022].
- The *Lift & Learn* method [Qian et al., 2019, Qian et al., 2020] and related work [Swischuk et al., 2020, Gosea and Antoulas, 2018, Jain and Kramer, 2021, McQuarrie et al., 2021], leverage lifting transformations for **learning low-order polynomial models** of complex nonlinear systems, such as combustion dynamics, from lifted data. For quadratic and cubic model structures, one can equip these learned ROMs with stability guarantees, see [Kramer, 2021, Sawant et al., 2023].
- **Equilibrium analysis** of geometrically nonlinear finite element models via quadratization [Guillot et al., 2019]

Variable transformations to improve modeling

Fluid mechanics:

- Symmetric variables to guarantee stable models [Hughes et al., 1986].
- Conservation properties via anti-symmetric variable transformations [Halpern et al., 2021]
- Model stabilization via specific volume variable representation [Balajewicz et al., 2016]
- Stability-preserving inner products with variable transformations [Kalashnikova and Barone, 2011, Rezaian and Wei, 2020].

Dynamical systems:

- Koopman operator and extended DMD [Williams et al., 2015, Netto et al., 2021].
- Canonical and abstract forms improve analysis [Liu et al., 2015, Brenig, 2018].
- [Savageau and Voit, 1987] showed that all ODE systems with (nested) elementary functions can be recast in a special polynomial system form, which is then faster to solve numerically.

Control design: Feedback linearization [Jakubczyk and Respondek, 1980, Khalil, 2002]

Definition of a Quadratization for PDEs

Consider a system of polynomial PDEs in unknown functions $u_1(t,x),\ldots,u_n(t,x)$ of the form

$$\partial_t y_i = p_i(\mathbf{y}, \partial_x \mathbf{y}, \ldots, \partial_x^h \mathbf{y}), \quad \text{for} \quad i = 1, 2, \ldots, n \tag{1}$$

where $p_1,\ldots,p_n \in \mathbb{C}[\mathbf{y}, \partial_x \mathbf{y}, \ldots, \partial_x^h \mathbf{y}]$. Consider a list of new variables

$$w_j = q_j(\mathbf{y}, \partial_x \mathbf{y}, \ldots, \partial_x^s \mathbf{y}), \quad \text{for} \quad j = 1, 2, \ldots, \ell$$

where s is an integer and $q_1,\ldots,q_\ell \in \mathbb{C}[\mathbf{y}, \partial_x \mathbf{y}, \ldots, \partial_x^s \mathbf{y}]$.

Then $w_1,\ldots,w_\ell$ are called a *quadratization* of (1) if there exist an integer H and polynomials $h_1,\ldots,h_{n+\ell} \in \mathbb{C}[\mathbf{y}, \mathbf{w}, \partial_x \mathbf{y}, \partial_x \mathbf{w}, \ldots, \partial_x^H \mathbf{y}, \partial_x^H \mathbf{w}]$ of total degree at most two such that

$$\partial_t y_i = h_i(\mathbf{y}, \mathbf{w}, \ldots, \partial_x^H \mathbf{y}, \partial_x^H \mathbf{w}) \quad \text{for every} \quad 1 \leqslant i \leqslant n \tag{2}$$

$$\partial_t w_j = h_{n+j}(\mathbf{y}, \mathbf{w}, \ldots, \partial_x^H \mathbf{y}, \partial_x^H \mathbf{w}) \quad \text{for every} \quad 1 \leqslant j \leqslant \ell \tag{3}$$

Theoretical results

Theorem (Existence of a PDE quadratization [Olivieri/Pogudin/K.,2026)

A PDE system of the form (1) *of order* h *has a monomial quadratization of differential order* $3h$.

Theorem (Complexity [Olivieri/Pogudin/K.,2026)

and [Hemery et al., 2020]] Finding an optimal monomial quadratization for a nonquadratic polynomial system of PDEs of the form (1) *is NP-hard.*

Can we automate this process? Which algorithms exist?

- Existence: **any set of ODEs with (nested) elementary functions can be polynomialized**. **Every polynomial system can be quadratized**; [Appelroth 1902, Lagutinskii 1911][Kerner, 1981, Carothers et al., 2005, Gu, 2011, Carravetta, 2015, Carravetta, 2020].
- **Implementation of those results would require introducing an excessively large number of variables**.
- The resulting quadratic systems can be pruned using constrained programming techniques; for polynomialization see [Hemery et al., 2021] and quadratization see [Hemery et al., 2020]. Both algorithms implemented in Biocham software
- In [Bychkov and Pogudin, 2021a] the quadratization problem for a polynomial system is framed as a tree exploration. The quadratization is obtained by building up the tree structure rather than pruning it as in [Hemery et al., 2020]. The resulting QBee [Bychkov and Pogudin, 2021b] algorithm has optimality guarantees for the dimension of the lifted system and good performance in practice [Bychkov and Pogudin, 2021a].

Our scientific discovery QuPDE algorithm

We developed a symbolic computing algorithm to find the **optimal** (smallest degree) **monomial** quadratization of a PDE [Olivieri et al., 2026].

- **Inputs**: 1) Symbolic form of the PDE; 2) additional knowledge to limit the search
- **Outputs**: 1) Symbolic quadratization variables; 2) final quadratic ODE

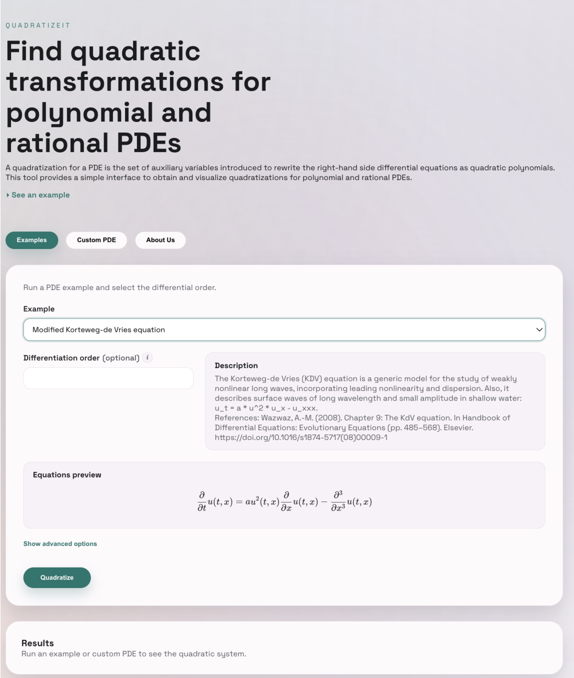
https://github.com/albaniolivieri/QuPDE

Functionalities

- Search monomials to reduce the search space
- Search can be limited to physically/mathematically realistic choices (e.g., enforcing regularity). Additional information accelerates the search.
- Handles rational functions as quadratization variables using Groebner reductions.
- Additional "pruning" rules (to eliminate branches of the search tree) can be added.

Results on common non-quadratic PDEs

PDE	Quadratization variables	CPU time	Nodes traversed
Solar wind model	$1/u$	8.8 ± 0.1 [ms]	1
Allen-Cahn equation	u^2	22.4 ± 0.1 [ms]	3
Schlögl model	u^2	43.8 ± 0.2 [ms]	3
Modified KdV	u^2	54.2 ± 0.9 [ms]	4
Euler equations	$1/\rho$	54.6 ± 1.1 [ms]	1
FHN system	v^2	115.1 ± 1.1 [ms]	3
Brusselator system	u^2, uv	129.6 ± 1.2 [ms]	8
Nonlinear heat equation	u^2, u^4, u^5	205.1 ± 2.5 [ms]	27
Schnakenberg equations	uv, u^2	445.0 ± 4.1 [ms]	8
Dym equation	u^3, $u_x^2 u$	628.9 ± 5.5 [ms]	21
Polynomial reaction ($d = 3$)	uv, v^2, $v^2 u$, v^3	9.9 ± 0.1 [s]	69
Polynomial reaction ($d = 4$)	uv, v^2, $v^2 u$, v^4, $v^3 u$	62.5 ± 0.4 [s]	305
Arrhenius-type reaction	$1/v$, $1/v^2$, uv, uy/v, uy/v^2, y/v, y/v^2	179.1 ± 0.4 [s]	491
Polynomial reaction ($d = 5$)	uv, v^2, v^3, $v^3 u$, $v^4 u$, v^5	636.1 ± 4.6 [s]	2107



Automated Software for Quadratization

quadratizeIt.com

- User-friendly interface (LaTeX source code as input and output)
- QuPDE algorithm in background (`https://github.com/albaniolivieri/QuPDE`
- PyPi Package: pip install qupde

A stroke of luck? The classic Cole-Hopf transformation

The Cole-Hopf transformation turns the quadratic Burgers' PDE into a linear PDE [Cole, 1951, Hopf, 1950]:

$$u_t(x,t) = \nu u_{xx}(x,t) - u(x,t)u_x(x,t); \qquad u(x,0) = u_0(x); \qquad u(0,t) = u(1,t) = 0.$$

Let's introduce a potential $\phi(x,t)$ such that $u(x,t) = \phi_x(x,t)$. The resulting equation is

$$\phi_{xt} = \nu\phi_{xxx} - \phi_x\phi_{xx} \qquad \xRightarrow{\text{Integrate}} \qquad \phi_t = \nu\phi_{xx} - \frac{1}{2}\phi_x^2$$

The Cole-Hopf nonlinear variable transformation

$$\phi = -2\nu\log(\psi) \quad \Rightarrow \qquad \phi_t = -\frac{2\nu}{\psi}\psi_t,\ \phi_x = -\frac{2\nu}{\psi}\psi_x, \quad \phi_{xx} = -\frac{2\nu}{\psi}\psi_{xx} + 2\nu\left(\frac{\psi_x}{\psi}\right)^2$$

The governing equation for the new variable ψ is just the linear heat equation:

$$\psi_t(x,t) = \nu\psi_{xx}(x,t) \quad \text{with initial condition} \quad \psi(x,0) = \exp\left(-\frac{1}{2\nu}\int_0^x u_0(z)\mathrm{d}z\right)$$

Key takeaways

Linearization $=$ Approximation

Quadratization $=$ Exact Reformulation

(and we can do it symbolically in software)

Part II:
Structure-preserving Lift & Learn

(combining lifting with model learning)

Lift & Learn for unstructured systems

1. **Given PDE, expose quadratic structure via lifting transformations [Qian et al., 2020]:**

$$\frac{\partial y(\mathbf{x},t)}{\partial t} = f(y(\mathbf{x},t)) \qquad \xrightarrow{\bar{y}=\tau_{\text{lift}}(y)} \qquad \frac{\partial \bar{y}(\mathbf{x},t)}{\partial t} = \mathcal{A}(\bar{y}(\mathbf{x},t)) + \mathcal{H}(\bar{y}(\mathbf{x},t)),$$

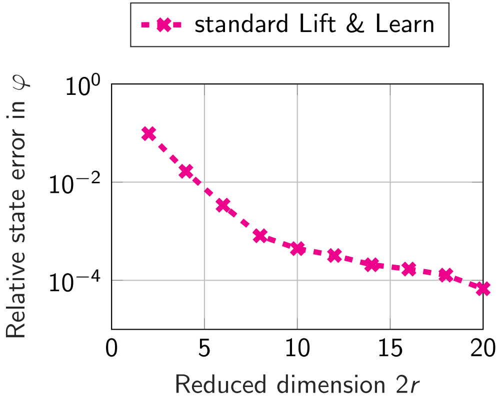
2. **Construct lifted training data:**
   - Simulate the original non-lifted FOM for K time steps to construct snapshot data $\mathbf{Y} \in \mathbb{R}^{n\times K}$
   - Obtain lifted snapshot data $\bar{\mathbf{Y}} \in \mathbb{R}^{\bar{n}\times K}$ from $\mathbf{Y} \in \mathbb{R}^{n\times K}$ via lifting map τ_{lift}
   - Construct a basis matrix $\bar{\mathbf{V}} \in \mathbb{R}^{\bar{n}\times \bar{r}}$ and then obtain the reduced snapshot data $\widehat{\mathbf{Y}}_r \in \mathbb{R}^{\bar{r}\times K}$
3. **Solve the least-squares problem via Operator Inference:**

$$\min_{\bar{\mathbf{A}}_r\in\mathbb{R}^{\bar{r}\times\bar{r}},\bar{\mathbf{H}}_r\in\mathbb{R}^{\bar{r}\times\bar{r}^2}} \|\dot{\widehat{\mathbf{Y}}}_r - \bar{\mathbf{A}}_r\widehat{\mathbf{Y}}_r - \bar{\mathbf{H}}_r(\widehat{\mathbf{Y}}_r \otimes \widehat{\mathbf{Y}}_r)\|_F$$

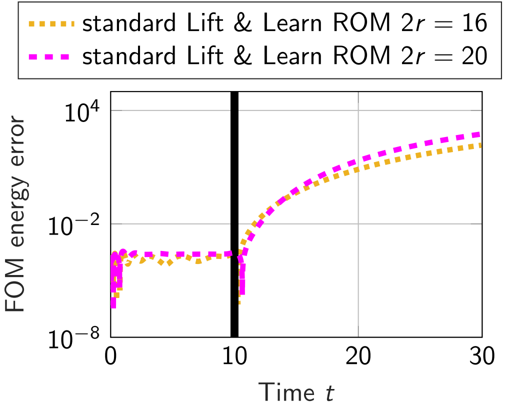
   to learn a quadratic ROM of a nonlinear FOM

$$\boxed{\dot{\bar{\mathbf{y}}}_r(t) = \bar{\mathbf{A}}_r\bar{\mathbf{y}}_r(t) + \bar{\mathbf{H}}_r(\bar{\mathbf{y}}_r(t) \otimes \bar{\mathbf{y}}_r(t))}$$

Standard Lift & Learn for sine-Gordon equation $\varphi_{tt} = \varphi_{xx} - \sin(\varphi)$



(a) Relative state error over the training data



(b) FOM energy error

Nonlinear PDEs with conservation laws

Consider conservative PDEs of the form

$$\frac{\partial^2 \phi(\mathbf{x}, t)}{\partial t^2} = \Delta \phi(\mathbf{x}, t) - f_{\text{non}}(\phi(\mathbf{x}, t)),$$

where $\mathbf{x} \in \mathbb{R}^d$ is the spatial variable, t is time, Δ is the Laplacian in $\mathbb{R}^d$, and $f_{\text{non}}(\phi(\mathbf{x}, t)) := \nabla_\phi(g(\phi(\mathbf{x}, t)))$, is derived from a smooth nonlinear function $g(\phi(\mathbf{x}, t))$.

The total energy is conserved for $t \geq 0$

$$\mathcal{E}[\phi(\mathbf{x}, t)] := \int_\Omega \left(\frac{1}{2} \left(\frac{\partial \phi(\mathbf{x}, t)}{\partial t} \right)^2 + \frac{1}{2} \left(\nabla \phi(\mathbf{x}, t) \right)^2 + g(\phi(\mathbf{x}, t)) \right) \mathrm{d}\mathbf{x}$$

The Hamiltonian case

Define $q(\mathbf{x},t) := \phi(\mathbf{x},t)$ and $p(\mathbf{x},t) := \frac{\partial}{\partial t}(\phi(\mathbf{x},t))$ to rewrite the PDE

$$\frac{\partial q(\mathbf{x},t)}{\partial t} = p(\mathbf{x},t), \qquad \frac{\partial p(\mathbf{x},t)}{\partial t} = \boldsymbol{\Delta} q(\mathbf{x},t) - f_{\text{non}}(q(\mathbf{x},t))$$

Spatial discretization leads to $2n-$dimensional nonlinear full-order model (FOM)

$$\dot{\mathbf{q}} = \mathbf{p}, \qquad \dot{\mathbf{p}} = \mathbf{D}\mathbf{q} - \mathbf{f}_{\text{non}}(\mathbf{q}),$$

where structure-preserving schemes ensure $\mathbf{D} = \mathbf{D}^\top \approx \Delta$

Nonlinear FOMs conserve the space-discretized energy

$$E(\mathbf{q},\mathbf{p}) = \frac{1}{2}\mathbf{p}^\top\mathbf{p} - \frac{1}{2}\mathbf{q}^\top\mathbf{D}\mathbf{q} + \sum_{i=1}^{n}(g(q_i))$$

Intrusive symplectic model reduction

- Symplectic projection using proper symplectic decomposition (PSD) basis $\mathbf{V}$

$$\begin{bmatrix} \mathbf{q} \\ \mathbf{p} \end{bmatrix} \approx \underbrace{\begin{bmatrix} \Phi & \mathbf{0} \\ \mathbf{0} & \Phi \end{bmatrix}}_{\mathbf{V}} \begin{bmatrix} \widehat{\mathbf{q}} \\ \widehat{\mathbf{p}} \end{bmatrix}$$

where $\Phi \in \mathbb{R}^{n \times r}$ is computed via SVD of $\mathbf{Y}_e := (\mathbf{Q}, \mathbf{P}) \in \mathbb{R}^{n \times 2K}$

- Structure-preserving reduced-order model (ROM) ([Peng and Mohseni, 2016])

$$\dot{\widehat{\mathbf{q}}} = \widehat{\mathbf{p}},$$
$$\dot{\widehat{\mathbf{p}}} = (\Phi^\top \mathbf{D} \Phi)\widehat{\mathbf{q}} - \Phi^\top \mathbf{f}_{\text{non}}(\Phi \widehat{\mathbf{q}})$$

conserves the nonlinear FOM energy exactly

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(E(\mathbf{V}\widehat{\mathbf{y}})\right) = 0$$

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- Structure-preserving reduced-order model (ROM) ([Peng and Mohseni, 2016])

$$\begin{aligned} \dot{\widehat{\mathbf{q}}} &= \widehat{\mathbf{p}}, \\ \dot{\widehat{\mathbf{p}}} &= (\Phi^\top \mathbf{D} \Phi) \widehat{\mathbf{q}} - \Phi^\top \mathbf{f}_{\text{non}}(\Phi \widehat{\mathbf{q}}) \end{aligned}$$

conserves the nonlinear FOM energy exactly

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(E(\mathbf{V}\widehat{\mathbf{y}}) \right) = 0$$

Drawback: Intrusive & nonlinearity requires extra (DEIM) approximation to speed up

Hamiltonian structure-preserving non-intrusive ROMs

1. Hamiltonian/Lagrangian Operator Inference ([Sharma et al., 2022], [Gruber and Tezaur, 2023], [Sharma and Kramer, 2024], [Geng et al., 2024], [Vijaywargiya et al., 2025])
   Drawback: Evaluation of $\Phi^\top \mathbf{f}_{\text{non}}(\Phi\widehat{\mathbf{q}})$ scales with the FOM dimension n
2. Hamiltonian Operator Inference combined with gradient-preserving discrete empirical interpolation method (DEIM) ([Wang, 2021], [Pagliantini et al., 2023])
   Drawback: Need to build and compute SVD of a Jacobian snapshot matrix of dimension $n \times rMK$ where M is the number of parameters
3. Lift & Learn ([Qian et al., 2019, 2020, 2022], [Swischuk et al., 2020], [Farcas et al., 2025])
   Drawback: Does not preserve the underlying geometric structure
4. Convolutional Autoencoder ROMs and SympNets for Hamiltonian Systems [Goyal et al., 2025]
   Drawback: FOM agnostic propagation model

Our goal: Learn a Hamiltonian ROM from data

Learning method requires three steps:

1. Find structure-preserving lifting variables that quadratize energy
2. Construct reduced snapshot data using the lifted map
3. Learn structure-preserving quadratic ROMs via constrained Operator Inference

Assumption: Have knowledge of the non-polynomial nonlinearity $\mathbf{f}_{\text{non}}(\mathbf{q})$ at the conservative PDE level.

Step 1: Structure-preserving lifting via energy quadratization

- Nonlinear conservative PDE with periodic boundary conditions

$$\frac{\partial q(\mathbf{x},t)}{\partial t} = p(\mathbf{x},t), \quad \frac{\partial p(\mathbf{x},t)}{\partial t} = \boldsymbol{\Delta} q(\mathbf{x},t) - f_{\text{non}}(q(\mathbf{x},t)),$$

with $f_{\text{non}}(q(\mathbf{x},t)) := \nabla_q (g(q(\mathbf{x},t))$

- The solution trajectories conserve the total energy

$$\mathcal{E}[q(\mathbf{x},t), p(\mathbf{x},t)] := \int_\Omega \left(\frac{1}{2} p(\mathbf{x},t)^2 + \frac{1}{2} \left(\nabla q(\mathbf{x},t)\right)^2 + g(q(\mathbf{x},t)) \right) \mathrm{d}\mathbf{x}.$$

- Define auxiliary variables as $w_1 = \tau_1(q) = \sqrt{g(q)}$ and $w_2 = \tau_2(q) = \frac{f_{\text{non}}(q)}{\sqrt{g(q)}}$

$$\frac{\partial p(\mathbf{x},t)}{\partial t} = \boldsymbol{\Delta} q(\mathbf{x},t) - w_1(\mathbf{x},t) w_2(\mathbf{x},t), \quad \frac{\partial w_1(\mathbf{x},t)}{\partial t} = \frac{f_{\text{non}}(q(\mathbf{x},t))}{2\sqrt{g(q(\mathbf{x},t))}} \frac{\partial q(\mathbf{x},t)}{\partial t} = \frac{1}{2} w_2(\mathbf{x},t) p(\mathbf{x},$$

Step 1: Structure-preserving lifting via energy quadratization

General Lifting Procedure:

- First two auxiliary variables w_1 and w_2 ensure that dynamics for $\{q, p, w_1\}$ are quadratic in terms of $\{q, p, w_1, w_2\}$, independent of nonlinear form of $g(q)$
- Compute auxiliary state dynamics for w_2 and if the dynamics are not quadratic in terms of the lifted variables $\{q, p, w_1, w_2\}$ then introduce another auxiliary variable w_3 that yields quadratic dynamics for w_2 in terms of the lifted variables $\{q, p, w_1, w_2, w_3\}$
- Continue this process of introducing auxiliary variables until we find a lifted PDE with quadratic dynamics in the lifted variables
  $\Rightarrow$ Existence of such a quadratization is a key assumption in our work

This approach leads to a lifted quadratic PDE with a finite number of auxiliary variables for all nonlinearities we considered (e.g., sinusoids, exponentials, etc)

Assuming this lifting strategy yields a quadratization with k auxiliary variables

$$
\begin{aligned}
\frac{\partial q(\mathbf{x},t)}{\partial t} &= p(\mathbf{x},t), \\
\frac{\partial p(\mathbf{x},t)}{\partial t} &= \boldsymbol{\Delta} q(\mathbf{x},t) - w_1(\mathbf{x},t) w_2(\mathbf{x},t), \\
\frac{\partial w_1(\mathbf{x},t)}{\partial t} &= \frac{1}{2} w_2(\mathbf{x},t) p(\mathbf{x},t), \\
\frac{\partial w_j(\mathbf{x},t)}{\partial t} &= \left(\alpha_j q(\mathbf{x},t) + \sum_{i=1}^{k} \alpha_{j,i} w_i(\mathbf{x},t) \right) p(\mathbf{x},t), \qquad \text{for} \qquad j = 2, \dots, k,
\end{aligned}
$$

where $\alpha_2, \dots, \alpha_k$ and $\alpha_{i,1}, \dots, \alpha_{i,k}$ for $i = 2, \dots, k$ are real-valued constant coefficients s.t. the constants in the set $\boldsymbol{\alpha}_i := \{\alpha_i, \alpha_{i,1}, \dots, \alpha_{i,k}\}$ can not be all zero.

This quadratic lifted PDE possesses a quadratic invariant in the lifted variables

$$
\mathcal{E}_{\text{lift}}[q(\mathbf{x},t), p(\mathbf{x},t), w_1(\mathbf{x},t), \cdots, w_k(\mathbf{x},t)] := \int_\Omega \left(\frac{1}{2} p(\mathbf{x},t)^2 + \frac{1}{2} \left(\nabla q(\mathbf{x},t) \right)^2 + w_1(\mathbf{x},t)^2 \right) \mathrm{d}\mathbf{x}
$$

Step 2: Constructing reduced snapshot data in the lifted setting

- Build the position and momentum snapshot data matrices

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

- Compute the lifted states as $\mathbf{w}_{i,j} = \tau_i(\mathbf{q}_j)$ and construct the lifted snapshot data matrix

$$\mathbf{W}_i = [\mathbf{w}_{i,1}, \cdots, \mathbf{w}_{i,K}] \in \mathbb{R}^{n \times K}, \qquad i = 1, \dots, k$$

- Use a block-diagonal basis matrix $\bar{\mathbf{V}} \in \mathbb{R}^{\bar{n} \times \bar{r}}$

$$\bar{\mathbf{V}} = \text{blkdiag}(\mathbf{\Phi}, \mathbf{\Phi}, \mathbf{V}_1, \cdots, \mathbf{V}_k) \in \mathbb{R}^{\bar{n} \times \bar{r}},$$

  where $\mathbf{\Phi}$ is the PSD basis matrix and $\mathbf{V}_i$ is the POD basis matrix

- Obtain projections of the snapshot data matrices as

$$\widehat{\mathbf{Q}} = \mathbf{\Phi}^\top \mathbf{Q} \in \mathbb{R}^{r \times K}, \qquad \widehat{\mathbf{P}} = \mathbf{\Phi}^\top \mathbf{P} \in \mathbb{R}^{r \times K}, \qquad \widehat{\mathbf{W}}_i = \mathbf{V}_i^\top \mathbf{W}_i \in \mathbb{R}^{r \times K}, \qquad i = 1, \dots, k$$

Step 3: Learning structure-preserving quadratic ROMs

- Postulate ROM form (following intrusive counterpart) as

$$\begin{aligned}
\dot{\widehat{\mathbf{q}}} &= \widehat{\mathbf{p}},\\
\dot{\widehat{\mathbf{p}}} &= \widehat{\mathbf{D}}\widehat{\mathbf{q}} + \color{blue}{\widehat{\mathbf{H}}_{\mathbf{p}}}(\widehat{\mathbf{w}}_1 \otimes \widehat{\mathbf{w}}_2),\\
\dot{\widehat{\mathbf{w}}}_1 &= \color{blue}{\widehat{\mathbf{H}}_{\mathbf{w}_1}}(\widehat{\mathbf{w}}_2 \otimes \widehat{\mathbf{p}}),\\
\dot{\widehat{\mathbf{w}}}_j &= \color{blue}{\widehat{\mathbf{H}}_{\mathbf{w}_j}}(\widehat{\mathbf{q}} \otimes \widehat{\mathbf{p}}) + \sum_{i=1}^{k} \color{blue}{\widehat{\mathbf{H}}_{\mathbf{w}_{j,i}}}(\widehat{\mathbf{w}}_i \otimes \widehat{\mathbf{p}}), \qquad \text{for} \qquad j = 2, \ldots, k.
\end{aligned}$$

- Key observation: $\color{blue}{\widehat{\mathbf{H}}_{\mathbf{p}}, \widehat{\mathbf{H}}_{\mathbf{w}_1}}$, and $\color{blue}{\widehat{\mathbf{H}}_{\mathbf{w}_j}, \widehat{\mathbf{H}}_{\mathbf{w}_{j,1}}, \cdots, \widehat{\mathbf{H}}_{\mathbf{w}_{j,k}}}$ for $j = 2, \ldots, k$ can be derived analytically ($\Rightarrow$ We *know* the lifting transformation!)

- Only need to infer $\widehat{\mathbf{D}}$ from

$$\widehat{\mathbf{D}} = \arg \min_{\widehat{\mathbf{D}} = \widehat{\mathbf{D}}^\top} \|\dot{\widehat{\mathbf{P}}} - \widehat{\mathbf{H}}_{\mathbf{p}}(\widehat{\mathbf{W}_1 \otimes \mathbf{W}_2}) - \widehat{\mathbf{D}}\widehat{\mathbf{Q}}\|_F.$$

Energy quadratization conserves lifted energy exactly

Assumption 1: The nonlinear potential energy component $g(q)$ is nonnegative.
Assumption 2: The proposed lifting strategy based on energy quadratization yields a quadratization of the nonlinear dynamics.

Theorem 1 ([Sharma/Draxl Giannoni/K., 2026])

Consider a nonlinear conservative FOM

$$\dot{\mathbf{q}} = \mathbf{p}, \qquad \dot{\mathbf{p}} = \mathbf{D}\mathbf{q} - \mathbf{f}_{\text{non}}(\mathbf{q}),$$

for which Assumptions 1 and 2 hold. Then, the proposed energy quadratization strategy combined with intrusive POD model reduction yields quadratic ROMs that conserve the lifted FOM energy exactly, i.e., $\frac{\mathrm{d}}{\mathrm{d}t}\left(E_{\text{lift}}\right) = 0$.

Proposition 1 ([Sharma/Draxl Giannoni/K., 2026])

The structure-preserving Lift & Learn ROM conserves the perturbed lifted FOM energy

$$\widehat{E}_{\text{lift}}(\widehat{\mathbf{q}}, \widehat{\mathbf{p}}, \widehat{\mathbf{w}}_1, \cdots, \widehat{\mathbf{w}}_k) := E_{\text{lift}}(\mathbf{\Phi}\widehat{\mathbf{q}}, \mathbf{\Phi}\widehat{\mathbf{p}}, \mathbf{V}_1\widehat{\mathbf{w}}_1, \cdots, \mathbf{V}_k\widehat{\mathbf{w}}_k) + \Delta E_{\text{lift}}(\widehat{\mathbf{q}})$$

with a perturbation $\Delta E_{\text{lift}}(\widehat{\mathbf{q}}) = \frac{1}{2}\widehat{\mathbf{q}}^\top(\mathbf{\Phi}^\top\mathbf{D}\mathbf{\Phi} - \widehat{\mathbf{D}})\widehat{\mathbf{q}}$ where $\mathbf{D} = \mathbf{D}^\top \in \mathbb{R}^{n\times n}$.

- The perturbation is bounded:

$$|\Delta E_{\text{lift}}(\widehat{\mathbf{q}})| = \frac{1}{2}\widehat{\mathbf{q}}^\top(\widetilde{\mathbf{D}} - \widehat{\mathbf{D}})\widehat{\mathbf{q}} \leq \frac{1}{2}\|\widetilde{\mathbf{D}} - \widehat{\mathbf{D}}\|\|\widehat{\mathbf{q}}\|^2,$$

  where $\widetilde{\mathbf{D}} := \mathbf{\Phi}^\top\mathbf{D}\mathbf{\Phi} \in \mathbb{R}^{r\times r}$ is the linear ROM operator obtained via intrusive projection.

Magnitude of the perturbation depends on the difference between the learned linear ROM operator $\widehat{\mathbf{D}}$ and the intrusively projected linear ROM operator $\widetilde{\mathbf{D}}$

Nonlinear conservative PDE

$$\frac{\partial^2 \phi(\mathbf{x},t)}{\partial t^2} = \boldsymbol{\Delta}\phi(\mathbf{x},t) - f_{\text{non}}(\phi(\mathbf{x},t))$$

Hamiltonian formulation

Nonlinear Hamiltonian PDE

$$\frac{\partial q(\mathbf{x},t)}{\partial t} = p(\mathbf{x},t)$$
$$\frac{\partial p(\mathbf{x},t)}{\partial t} = \boldsymbol{\Delta} q(\mathbf{x},t) - f_{\text{non}}(q(\mathbf{x},t))$$

Requires:
1. FOM snapshot data
2. PDE knowledge

Hamiltonian Operator Inference

Data-driven nonlinear ROM
structure-preserving
computationally inefficient

Requires:
1. Jacobian snapshot data

Structure-preserving hyper-reduction

Data-driven nonlinear ROM
structure-preserving
computationally efficient

Lifting via energy quadratization

Lifted quadratic PDE

$$\frac{\partial q(\mathbf{x},t)}{\partial t} = p(\mathbf{x},t)$$
$$\frac{\partial p(\mathbf{x},t)}{\partial t} = \boldsymbol{\Delta} q(\mathbf{x},t) - w_1(\mathbf{x},t) w_2(\mathbf{x},t)$$
$$\frac{\partial w_1(\mathbf{x},t)}{\partial t} = \frac{1}{2} w_2(\mathbf{x},t) p(\mathbf{x},t)$$
$$\frac{\partial w_j(\mathbf{x},t)}{\partial t} = \left(\alpha_j q(\mathbf{x},t) + \sum_{i=1}^{k} \alpha_{j,i} w_i(\mathbf{x},t)\right) p(\mathbf{x},t)$$

Requires:
1. FOM snapshot data
2. PDE knowledge

Structure-preserving Lift & Learn

Data-driven quadratic ROM
structure-preserving
computationally efficient
no additional hyper-reduction

Numerical examples

- The *relative state error* in q is computed in the entire training or testing intervals:

$$\text{Relative state error in } q = \frac{\|\mathbf{Q} - \mathbf{\Phi}\widehat{\mathbf{Q}}\|_F^2}{\|\mathbf{Q}\|_F^2},$$

  where $\widehat{\mathbf{Q}} = [\widehat{\mathbf{q}}_1, \cdots, \widehat{\mathbf{q}}_K] \in \mathbb{R}^{r \times K}$ is the ROM snapshot data obtained from the ROM simulations and $\mathbf{\Phi}\widehat{\mathbf{Q}} \in \mathbb{R}^{n \times K}$ is the approximation of the FOM data $\mathbf{Q}$
- We measure the common cost/accuracy tradeoff for ROMs using *efficacy:*

$$\text{Efficacy} = \frac{1}{\text{relative state error in training data regime} \times \text{wall-clock time in seconds}}$$

- The *FOM energy error* is computed as follows:

$$\text{FOM energy error} = |E(\mathbf{\Phi}\widehat{\mathbf{q}}(t), \mathbf{\Phi}\widehat{\mathbf{p}}(t)) - E(\mathbf{\Phi}\widehat{\mathbf{q}}(0), \mathbf{\Phi}\widehat{\mathbf{p}}(0))|$$

Two-dimensional Klein-Gordon-Zakharov (KGZ) equation

- Describe interaction between Langmuir waves and ion acoustic waves in plasma
- Governing PDEs with periodic boundary conditions

$$\psi_{tt} = \Delta\psi - \psi - \psi\phi - |\psi|^2\psi, \quad \phi_{tt} = \Delta\phi + \Delta(|\psi|^2)$$

where $\psi(\mathbf{x}, t)$ is a complex-valued function and $\phi(\mathbf{x}, t)$ is a real-valued function.

- The coupled system of PDEs conserves the total energy

$$E(t) = \int \left(\left| \frac{\partial \psi}{\partial t} \right|^2 + |\nabla\psi|^2 + |\psi|^2 + \phi|\psi|^2 + \frac{|\nabla\varphi|^2}{2} + \frac{\phi^2}{2} + \frac{|\psi|^4}{2} \right) \mathrm{d}\mathbf{x},$$

where $\varphi(\mathbf{x}, t)$ is defined via $\Delta\varphi(\mathbf{x}, t) = \phi_t$ with $\lim_{|x|\to\infty} \varphi = 0$

Structure-preserving lifting for Klein-Gordon-Zakharov Equation

Nonlinear conservative FOM

$$
\begin{aligned}
\dot{\mathbf{q}}_1 &= \mathbf{p}_1, \\
\dot{\mathbf{q}}_2 &= \mathbf{p}_2 \\
\dot{\mathbf{p}}_1 &= \mathbf{D}\mathbf{q}_1 - \mathbf{q}_1 - \boldsymbol{\phi} \odot \mathbf{q}_1 - (\mathbf{q}_1^2 + \mathbf{q}_2^2)\mathbf{q}_1 \\
\dot{\mathbf{p}}_2 &= \mathbf{D}\mathbf{q}_2 - \mathbf{q}_2 - \boldsymbol{\phi} \odot \mathbf{q}_2 - (\mathbf{q}_1^2 + \mathbf{q}_2^2)\mathbf{q}_2 \\
\dot{\boldsymbol{\varphi}} &= \boldsymbol{\phi} + (\mathbf{q}_1^2 + \mathbf{q}_2^2) \\
\dot{\boldsymbol{\phi}} &= \mathbf{D}\boldsymbol{\varphi}
\end{aligned}
$$

$$
\begin{aligned}
E = {} & \mathbf{p}_1^\top \mathbf{p}_1 + \mathbf{p}_2^\top \mathbf{p}_2 + \mathbf{q}_1^\top \mathbf{q}_1 + \mathbf{q}_2^\top \mathbf{q}_2 \\
& - \mathbf{q}_1^\top \mathbf{D}\mathbf{q}_1 - \mathbf{q}_2^\top \mathbf{D}\mathbf{q}_2 + \boldsymbol{\phi}^\top(\mathbf{q}_1^2 + \mathbf{q}_2^2) - \frac{1}{2}\boldsymbol{\varphi}^\top \mathbf{D}\boldsymbol{\varphi} \\
& + \frac{1}{2}\boldsymbol{\phi}^\top \boldsymbol{\phi} + \frac{1}{2}(\mathbf{q}_1^2 + \mathbf{q}_2^2)^2
\end{aligned}
$$

Structure-preserving lifting for Klein-Gordon-Zakharov Equation

Nonlinear conservative FOM

$$
\begin{aligned}
\dot{\mathbf{q}}_1 &= \mathbf{p}_1,\\
\dot{\mathbf{q}}_2 &= \mathbf{p}_2\\
\dot{\mathbf{p}}_1 &= \mathbf{D}\mathbf{q}_1 - \mathbf{q}_1 - \boldsymbol{\phi}\odot\mathbf{q}_1 - (\mathbf{q}_1^2+\mathbf{q}_2^2)\mathbf{q}_1\\
\dot{\mathbf{p}}_2 &= \mathbf{D}\mathbf{q}_2 - \mathbf{q}_2 - \boldsymbol{\phi}\odot\mathbf{q}_2 - (\mathbf{q}_1^2+\mathbf{q}_2^2)\mathbf{q}_2\\
\dot{\boldsymbol{\varphi}} &= \boldsymbol{\phi} + (\mathbf{q}_1^2+\mathbf{q}_2^2)\\
\dot{\boldsymbol{\phi}} &= \mathbf{D}\boldsymbol{\varphi}
\end{aligned}
$$

$$\xrightarrow{\mathbf{w}=\mathbf{q}_1^2+\mathbf{q}_2^2}$$

$$
\begin{aligned}
E = {} & \mathbf{p}_1^\top\mathbf{p}_1 + \mathbf{p}_2^\top\mathbf{p}_2 + \mathbf{q}_1^\top\mathbf{q}_1 + \mathbf{q}_2^\top\mathbf{q}_2\\
& - \mathbf{q}_1^\top\mathbf{D}\mathbf{q}_1 - \mathbf{q}_2^\top\mathbf{D}\mathbf{q}_2 + \boldsymbol{\phi}^\top(\mathbf{q}_1^2+\mathbf{q}_2^2) - \frac{1}{2}\boldsymbol{\varphi}^\top\mathbf{D}\boldsymbol{\varphi}\\
& + \frac{1}{2}\boldsymbol{\phi}^\top\boldsymbol{\phi} + \frac{1}{2}(\mathbf{q}_1^2+\mathbf{q}_2^2)^2
\end{aligned}
$$

Structure-preserving lifting for Klein-Gordon-Zakharov Equation

Nonlinear conservative FOM

$$
\begin{aligned}
\dot{\mathbf{q}}_1 &= \mathbf{p}_1, \\
\dot{\mathbf{q}}_2 &= \mathbf{p}_2 \\
\dot{\mathbf{p}}_1 &= \mathbf{D}\mathbf{q}_1 - \mathbf{q}_1 - \boldsymbol{\phi} \odot \mathbf{q}_1 - (\mathbf{q}_1^2 + \mathbf{q}_2^2)\mathbf{q}_1 \\
\dot{\mathbf{p}}_2 &= \mathbf{D}\mathbf{q}_2 - \mathbf{q}_2 - \boldsymbol{\phi} \odot \mathbf{q}_2 - (\mathbf{q}_1^2 + \mathbf{q}_2^2)\mathbf{q}_2 \\
\dot{\boldsymbol{\varphi}} &= \boldsymbol{\phi} + (\mathbf{q}_1^2 + \mathbf{q}_2^2) \\
\dot{\boldsymbol{\phi}} &= \mathbf{D}\boldsymbol{\varphi}
\end{aligned}
$$

$$\xrightarrow{\mathbf{w} = \mathbf{q}_1^2 + \mathbf{q}_2^2}$$

Equivalent quadratic FOM

$$
\begin{aligned}
\dot{\mathbf{q}}_1 &= \mathbf{p}_1, \\
\dot{\mathbf{q}}_2 &= \mathbf{p}_2, \\
\dot{\mathbf{p}}_1 &= \mathbf{D}\mathbf{q}_1 - \mathbf{q}_1 - \boldsymbol{\phi} \odot \mathbf{q}_1 - \mathbf{w} \odot \mathbf{q}_1, \\
\dot{\mathbf{p}}_2 &= \mathbf{D}\mathbf{q}_2 - \mathbf{q}_2 - \boldsymbol{\phi} \odot \mathbf{q}_2 - \mathbf{w} \odot \mathbf{q}_2, \\
\dot{\boldsymbol{\varphi}} &= \boldsymbol{\phi} + \mathbf{w}, \\
\dot{\boldsymbol{\phi}} &= \mathbf{D}\boldsymbol{\varphi}, \\
\dot{\mathbf{w}} &= 2\mathbf{q}_1 \odot \mathbf{p}_1 + 2\mathbf{q}_2 \odot \mathbf{p}_2,
\end{aligned}
$$

$$
\begin{aligned}
E = &\ \mathbf{p}_1^\top \mathbf{p}_1 + \mathbf{p}_2^\top \mathbf{p}_2 + \mathbf{q}_1^\top \mathbf{q}_1 + \mathbf{q}_2^\top \mathbf{q}_2 \\
&- \mathbf{q}_1^\top \mathbf{D}\mathbf{q}_1 - \mathbf{q}_2^\top \mathbf{D}\mathbf{q}_2 + \boldsymbol{\phi}^\top(\mathbf{q}_1^2 + \mathbf{q}_2^2) - \frac{1}{2}\boldsymbol{\varphi}^\top \mathbf{D}\boldsymbol{\varphi} \\
&+ \frac{1}{2}\boldsymbol{\phi}^\top \boldsymbol{\phi} + \frac{1}{2}(\mathbf{q}_1^2 + \mathbf{q}_2^2)^2
\end{aligned}
$$

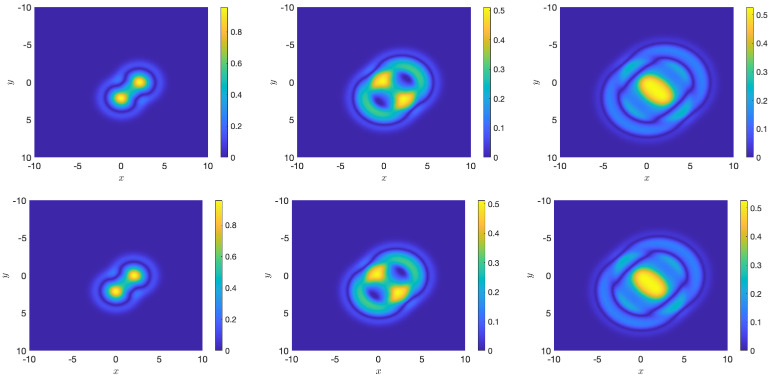
$$
\begin{aligned}
E_{\text{lift}} = &\ \mathbf{p}_1^\top \mathbf{p}_1 + \mathbf{p}_2^\top \mathbf{p}_2 + \mathbf{q}_1^\top \mathbf{q}_1 + \mathbf{q}_2^\top \mathbf{q}_2 \\
&- \mathbf{q}_1^\top \mathbf{D}\mathbf{q}_1 - \mathbf{q}_2^\top \mathbf{D}\mathbf{q}_2 + \boldsymbol{\phi}^\top \mathbf{w} - \frac{1}{2}\boldsymbol{\varphi}^\top \mathbf{D}\boldsymbol{\varphi} \\
&+ \frac{1}{2}\boldsymbol{\phi}^\top \boldsymbol{\phi} + \frac{1}{2}\mathbf{w}^\top \mathbf{w}
\end{aligned}
$$

$|\psi(x,y)|$ predictions with sp Lift & Learn ROM of dime. $7r = 140$

FOM dimension $6n = 960,000$; Training data $[0,4]$; Test data $[4,5]$

Conservative FOM

sp Lift & Learn ROM

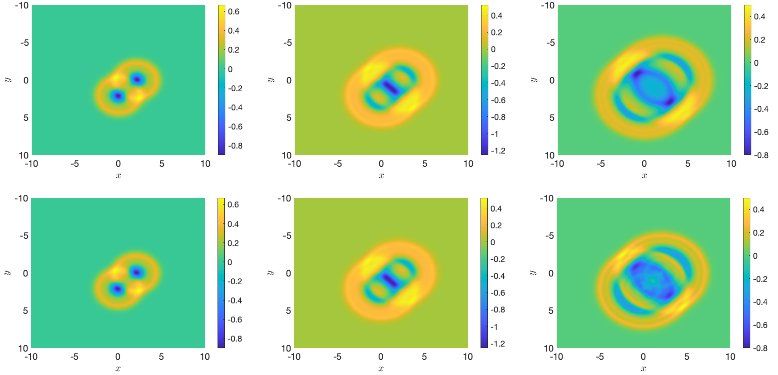


(a) $t = 1.5$ **(b)** $t = 3$ **(c)** $t = 4.5$

$\phi(x, y)$ predictions with sp Lift & Learn ROM of dim. $7r = 140$

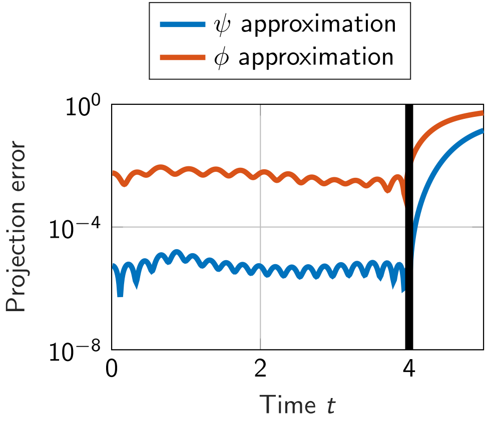
Conservative FOM

sp Lift & Learn ROM

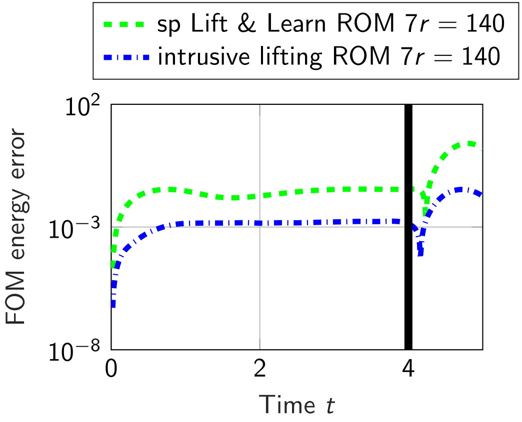


(a) $t = 1.5$ **(b)** $t = 3$ **(c)** $t = 4.5$

Projection error and FOM energy error



(a) Projection error



(b) FOM energy error

Concluding remarks

Variable transformations

- Can identify new structures in PDEs and ODEs
- Are beneficial as a pre-processing step to enable learning
- Symbolic search produces exact transformations

Structure-preserving Lift & Learn for nonlinear wave equations

- Grey Box: leverages knowledge about PDE, but not its discretization, to enforce physics preservation in the learning process
- achieves accuracy and computational efficiency similar to Hamiltonian Operator Inference with structure-preserving DEIM
- can be flexibly adapted to learn structure-preserving quadratic ROMs for a wider class of coupled conservative PDEs

Future work

1. Embedding physical constraints into optimal quadratization techniques
2. Address boundary conditions and uniqueness for the PDE case

Thank you!

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