



The University of Texas at Austin

Oden Institute for Computational
Engineering and Sciences

Projection-based Model Reduction

Formulations for Physics-based Machine Learning

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Oden Institute for Computational Engineering and Sciences

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SIAM CSE19

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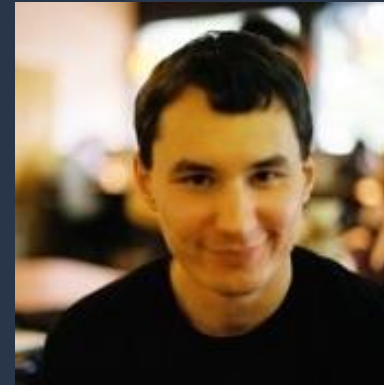


ODEN INSTITUTE

TRANSFORMING COMPUTING
FOR SCIENCE, ENGINEERING & MEDICINE

Contributors

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Physics-based models have structure

But they are large-scale and expensive to solve, and often embodied in black-box solvers

Consider physics-based models represented as systems of ODEs or spatial discretization of PDEs describing the system of interest

- which in turn arise from governing physical principles (conservation laws, etc.)

$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{A}(\mathbf{p})\mathbf{x} + \mathbf{B}(\mathbf{p})\mathbf{u} \\ \mathbf{y} &= \mathbf{C}(\mathbf{p})\mathbf{x}\end{aligned}$$

$$\begin{aligned}\dot{\mathbf{x}} &= f(\mathbf{x}, \mathbf{p}, \mathbf{u}) \\ \mathbf{y} &= g(\mathbf{x}, \mathbf{p}, \mathbf{u})\end{aligned}$$

$\mathbf{x} \in \mathbf{R}^N$: state vector

$\mathbf{u} \in \mathbf{R}^{N_i}$: input vector

$\mathbf{p} \in \mathbf{R}^{N_p}$: parameter vector

$\mathbf{y} \in \mathbf{R}^{N_o}$: output vector

Projection preserves structure

Reduced models:
Low-cost but accurate approximations of high-fidelity models via projection onto a low-dimensional subspace

Interpretable & analyzable

$$\begin{array}{l} \dot{\mathbf{x}} = \mathbf{A}(\mathbf{p})\mathbf{x} + \mathbf{B}(\mathbf{p})\mathbf{u} \\ \mathbf{y} = \mathbf{C}(\mathbf{p})\mathbf{x} \end{array} \xrightarrow{\mathbf{x} \approx \mathbf{V}\mathbf{x}_r} \begin{array}{l} \mathbf{r} = \mathbf{V}\dot{\mathbf{x}}_r - \mathbf{A}\mathbf{V}\mathbf{x}_r - \mathbf{B}\mathbf{u} \\ \mathbf{y}_r = \mathbf{C}\mathbf{V}\mathbf{x}_r \end{array}$$

FOM

$$\downarrow \mathbf{W}^T \mathbf{r} = 0$$

$$\begin{aligned} \mathbf{A}_r(\mathbf{p}) &= \mathbf{W}^T \mathbf{A}(\mathbf{p}) \mathbf{V} \\ \mathbf{B}_r(\mathbf{p}) &= \mathbf{W}^T \mathbf{B}(\mathbf{p}) \\ \mathbf{C}_r(\mathbf{p}) &= \mathbf{C}(\mathbf{p}) \mathbf{V} \end{aligned}$$

$$\begin{array}{l} \dot{\mathbf{x}}_r = \mathbf{A}_r(\mathbf{p})\mathbf{x}_r + \mathbf{B}_r(\mathbf{p})\mathbf{u} \\ \mathbf{y}_r = \mathbf{C}_r(\mathbf{p})\mathbf{x}_r \end{array}$$

ROM

$\mathbf{x} \in \mathbf{R}^N$: state vector
 $\mathbf{p} \in \mathbf{R}^{N_p}$: parameter vector
 $\mathbf{u} \in \mathbf{R}^{N_i}$: input vector
 $\mathbf{y} \in \mathbf{R}^{N_o}$: output vector

$\mathbf{x}_r \in \mathbf{R}^n$: reduced state vector
 $\mathbf{V} \in \mathbf{R}^{N \times n}$: reduced basis

What is the connection between reduced order modeling and machine learning?

Machine learning

“Machine learning is a field of computer science that uses statistical techniques to give computer systems the ability to "learn" with data, without being explicitly programmed.” [Wikipedia]

Reduced order modeling

“Model order reduction (MOR) is a technique for reducing the computational complexity of mathematical models in numerical simulations.” [Wikipedia]

The difference in fields is perhaps largely one of history and perspective: model reduction methods have grown from the scientific computing community, with a focus on *reducing* high-dimensional models that arise from physics-based modeling, whereas machine learning has grown from the computer science community, with a focus on *creating* low-dimensional models from black-box data streams. Yet recent years have seen an increased blending of the two perspectives and a recognition of the associated opportunities. [Swischuk et al., *Computers & Fluids*, 2018]

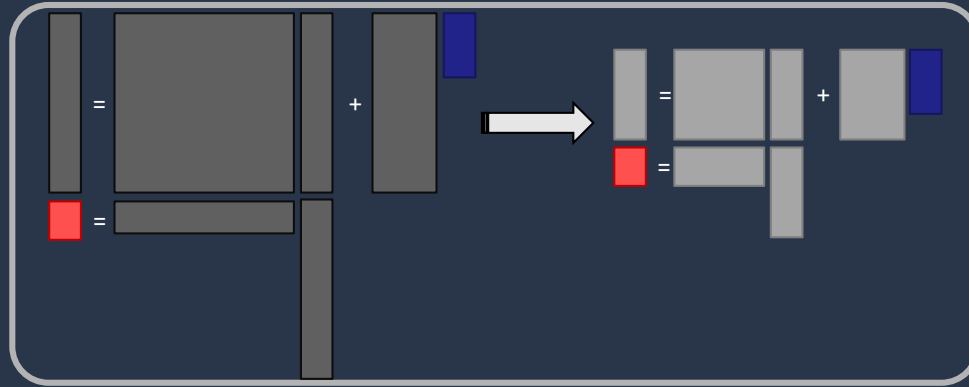
Outline

domain-aware
interpretable
analyzable

1. Reduced models can be learned from data
2. Basis expansions can be constructed so as to respect physical constraints
3. Structure can be exposed through variable transformations

This work was supported in part by the U.S. Air Force **Center of Excellence on Multi-Fidelity Modeling of Rocket Combustor Dynamics**, the AFOSR MURI on **Managing Multiple Information Sources of Multi-physics Systems**, the U.S. Department of Energy Applied Mathematics program as part of the **DiaMonD Multifaceted Mathematics Integrated Capability Center**, the AFOSR **Dynamic Data Driven Application System Program**, and the **MIT-SUTD International Design Center**.





1. Reduced models can be learned from data

Given state snapshot data (simulation or experimental), learn the dynamical system that (may have) generated it

Linear Model

$$\text{FOM: } \mathbf{E}\dot{\mathbf{x}} = \underbrace{\mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u}}_{\text{linear}}$$

$$\text{ROM: } \hat{\mathbf{E}}\dot{\hat{\mathbf{x}}} = \hat{\mathbf{A}}\hat{\mathbf{x}} + \hat{\mathbf{B}}\mathbf{u}$$

ROM preserves linear structure:

$$\hat{\mathbf{A}} = \mathbf{V}^\top \mathbf{A} \mathbf{V}, \quad \hat{\mathbf{B}} = \mathbf{V}^\top \mathbf{B}, \quad \hat{\mathbf{E}} = \mathbf{V}^\top \mathbf{E} \mathbf{V}$$

Quadratic Model

$$\text{FOM: } \mathbf{E}\dot{\mathbf{x}} = \underbrace{\mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u}}_{\text{linear}} + \underbrace{\mathbf{H}(\mathbf{x} \otimes \mathbf{x})}_{\text{quadratic}}$$

$$\text{ROM: } \hat{\mathbf{E}}\dot{\hat{\mathbf{x}}} = \hat{\mathbf{A}}\hat{\mathbf{x}} + \hat{\mathbf{B}}\mathbf{u} + \hat{\mathbf{H}}(\hat{\mathbf{x}} \otimes \hat{\mathbf{x}})$$

ROM preserves quadratic structure:

$$\hat{\mathbf{H}} = \mathbf{V}^\top \mathbf{H}(\mathbf{V} \otimes \mathbf{V})$$

Projection-based model reduction gives us the mathematical lens through which to learn physics-based low-dimensional models from data

Given state data, learn the system

Operator Inference

Peherstorfer & W.
Data-driven operator inference for nonintrusive projection-based model reduction, *Computer Methods in Applied Mechanics and Engineering*, 2016

$$\mathbf{E}\dot{\mathbf{x}} = \underbrace{\mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u}}_{\text{linear}} + \underbrace{\mathbf{H}(\mathbf{x} \otimes \mathbf{x})}_{\text{quadratic}}$$

Given state data (\mathbf{X}) and velocity data ($\dot{\mathbf{X}}$):

$$\mathbf{X} = \begin{bmatrix} | & & | \\ \mathbf{x}(t_1) & \dots & \mathbf{x}(t_K) \\ | & & | \end{bmatrix} \quad \dot{\mathbf{X}} = \begin{bmatrix} | & & | \\ \dot{\mathbf{x}}(t_1) & \dots & \dot{\mathbf{x}}(t_K) \\ | & & | \end{bmatrix}$$

Find the operators \mathbf{A} , \mathbf{B} , \mathbf{E} , \mathbf{H}
by solving the least squares problem:

$$\min_{\mathbf{A}, \mathbf{B}, \mathbf{E}, \mathbf{H}} \left\| \mathbf{X}^T \mathbf{A}^T + (\mathbf{X} \otimes \mathbf{X})^T \mathbf{H}^T + \mathbf{U}^T \mathbf{B}^T - \dot{\mathbf{X}}^T \mathbf{E} \right\|$$

Learning a low-dimensional system

In a global basis, here via the proper orthogonal decomposition (POD)

Operator Inference [Peherstorfer & Willcox, 2016]

1. Generate full state trajectories (from high-fidelity simulation)

$$\mathbf{X} = \begin{bmatrix} | & & | \\ \mathbf{x}(t_1) & \dots & \mathbf{x}(t_K) \\ | & & | \end{bmatrix} \quad \dot{\mathbf{X}} = \begin{bmatrix} | & & | \\ \dot{\mathbf{x}}(t_1) & \dots & \dot{\mathbf{x}}(t_K) \\ | & & | \end{bmatrix}$$

Learning a low-dimensional system

In a global basis,
here via the
proper orthogonal
decomposition (POD)

Operator Inference [Peherstorfer & Willcox, 2016]

1. Generate full state trajectories
(from high-fidelity simulation)
2. Compute POD basis from these trajectories

$$\mathbf{X} = \mathbf{V} \mathbf{\Sigma} \mathbf{W}^T$$

Learning a low-dimensional system

In a global basis, here via the proper orthogonal decomposition (POD)

Operator Inference [Peherstorfer & Willcox, 2016]

1. Generate full state trajectories (from high-fidelity simulation)
2. Compute POD basis from these trajectories
3. Project trajectories onto POD basis, to obtain trajectories in low-dimensional POD coordinate space

$$\hat{\mathbf{X}} = \mathbf{V}^T \mathbf{X}$$

Learning a low-dimensional system

In a global basis, here via the proper orthogonal decomposition (POD)

Operator Inference [Peherstorfer & Willcox, 2016]

1. Generate full state trajectories (from high-fidelity simulation)
2. Compute POD basis from these trajectories
3. Project trajectories onto POD basis, to obtain trajectories in low-dimensional POD coordinate space
4. Solve least squares minimization problem to infer the low-dimensional model

$$\min_{\hat{\mathbf{A}}, \hat{\mathbf{B}}, \hat{\mathbf{E}}, \hat{\mathbf{H}}} \left\| \hat{\mathbf{X}}^T \hat{\mathbf{A}}^T + (\hat{\mathbf{X}} \otimes \hat{\mathbf{X}})^T \hat{\mathbf{H}}^T + \mathbf{U}^T \hat{\mathbf{B}}^T - \dot{\hat{\mathbf{X}}}^T \hat{\mathbf{E}} \right\|$$

Learning a low-dimensional system

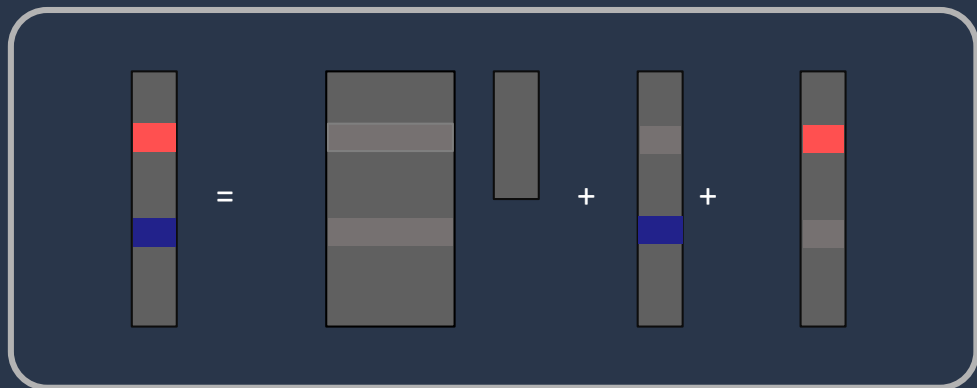
In a global basis, here via the proper orthogonal decomposition (POD)

Operator Inference [Peherstorfer & Willcox, 2016]

1. Generate full state trajectories (from high-fidelity simulation)
2. Compute POD basis from these trajectories
3. Project trajectories onto POD basis, to obtain trajectories in low-dimensional POD coordinate space
4. Solve least squares minimization problem to infer the low-dimensional model

Under certain conditions, recovers the intrusive POD reduced model

→ **convenience** of black-box learning +
rigor of projection-based reduction +
structure imposed by physics



2. Basis expansions can be constructed so as to respect physical constraints

Using particular solutions to enforce constraints by construction

Representing a high-dimensional state in a low-dimensional basis

$$\mathbf{x}(t) \approx \mathbf{V} \hat{\mathbf{x}}(t) = \sum_{i=1}^r \mathbf{V}_i \hat{x}_i(t)$$

Proper orthogonal decomposition (POD):

- Basis vectors \mathbf{V}_i are linear combinations of snapshots
- If snapshots satisfy homogeneous conditions (e.g., BCs, divergence, etc.)
 - basis vectors satisfy those conditions
 - reconstructed solution satisfies conditions

We can enforce other (non-homogeneous) conditions using particular solutions

$\bar{\mathbf{x}}(t)$: particular solution chosen to enforce a desired condition

$$\mathbf{x} \approx \bar{\mathbf{x}}(t) + \mathbf{V} \hat{\mathbf{x}}(t) = \bar{\mathbf{x}}(t) + \underbrace{\sum_{i=1}^r \mathbf{V}_i \hat{x}_i(t)}_{\text{solution satisfies desired condition by construction}}$$

basis functions modified to be homogeneous wrt the desired condition

solution satisfies desired condition by construction

Computing particular solutions

Also known in model reduction literature as “static corrections”

Romanowski & Dowell, 1994;
Hall, Thomas & Dowell, 2000;
Willcox, 2000

Simple example: representing the temperature profile $T(z, t)$ in a 1D heated rod



$$\text{BCs: } T(0, t) = \gamma_0 f(t)$$

$$T(L, t) = \gamma_L$$

Auxiliary problem 1: solution $\bar{T}^L(z)$



$$\text{BCs: } T(0, t) = 0$$

$$T(L, t) = 1$$

Auxiliary problem 2: solution $\bar{T}^0(z)$



$$\text{BCs: } T(0, t) = 1$$

$$T(L, t) = 0$$

Particular solutions

used to enforce non-homogeneous boundary conditions

Swischuk, Mainini,
Peherstorfer & W.,
Computers & Fluids, 2018

- Modify snapshots to satisfy homogenous BCs:

$$\tilde{T}(z, t_j) = T(z, t_j) - \underbrace{\gamma_0 f(t_j) \bar{T}^0(z) - \gamma_L \bar{T}^L(z)}_{\text{particular solutions scaled by the BC for that snapshot}}$$

particular solutions scaled
by the BC for that snapshot

- POD basis vectors $V_i, i = 1, \dots, r$ computed from modified snapshots satisfy homogeneous conditions
- Temperature solution expanded in POD basis with modal coefficients $\hat{T}_i, i = 1, \dots, r$
- Reconstructed solution:

$$T(x, t) = \underbrace{\gamma_0 f(t) \bar{T}^0(z) - \gamma_L \bar{T}^L(z)}_{\text{enforces a specified set of BCs}} + \underbrace{\sum_{i=1}^r V_i(z) \hat{T}_i(t)}_{\text{satisfies homogeneous BCs}}$$

enforces a specified
set of BCs

satisfies
homogeneous BCs

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (E + p)u \end{pmatrix} = 0$$

$$E = \frac{p}{\gamma - 1} + \frac{1}{2} \rho u^2$$

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ u \\ p \end{pmatrix} + \begin{pmatrix} \rho \frac{\partial u}{\partial x} + u \frac{\partial \rho}{\partial x} \\ u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} \\ \gamma p \frac{\partial u}{\partial x} + \frac{\partial}{\partial t} \begin{pmatrix} u \\ p \\ q \end{pmatrix} \end{pmatrix} + \begin{pmatrix} u \frac{\partial u}{\partial x} + q \frac{\partial p}{\partial x} \\ \gamma p \frac{\partial u}{\partial x} + u \frac{\partial p}{\partial x} \\ q \frac{\partial u}{\partial x} + u \frac{\partial q}{\partial x} \end{pmatrix} = 0$$

3. Lifting

Structure can be exposed through variable transformations

Very simple example

Lifting a 4th-order ODE to quadratic-bilinear form.

Can either lift to a system of ODEs or to a system of DAEs

Consider the fourth order system

$$\dot{x} = x^4 + u.$$

Introduce auxiliary variables:

$$w_1 = x^2 \quad w_2 = w_1^2$$

Chain rule:

$$\dot{w}_1 = 2x[w_1^2 + u] = 2x[w_2 + u]$$

$$\dot{w}_2 = 2w_1\dot{w}_1 = 4xw_1[w_2 + u]$$

Need additional variable to make auxiliary dynamics quadratic:

$$\begin{aligned} w_3 &= xw_1 & \dot{w}_3 &= \dot{x}w_1 + x\dot{w}_1 \\ & & &= w_1w_2 + w_1u + 2w_1w_2 + 2w_1u \end{aligned}$$

QB-ODE

$$\begin{aligned} \dot{x} &= w_2 + u \\ \dot{w}_1 &= 2xw_2 + 2xu \\ \dot{w}_2 &= 4w_2w_3 + 4w_3u \\ \dot{w}_3 &= 3w_1w_2 + 3w_1u \end{aligned}$$

QB-DAE

$$\begin{aligned} \dot{x} &= w_1^2 + u \\ 0 &= w_1 - x^2 \end{aligned}$$

Lifting example: Euler equations

Transformation to
specific volume form
(use $1/\rho$ in place of ρ)
yields a quadratic
system of ODEs

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (E + p)u \end{pmatrix} = 0$$

$$E = \frac{p}{\gamma - 1} + \frac{1}{2} \rho u^2$$

conservative variables

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ u \\ p \end{pmatrix} + \begin{pmatrix} \rho \frac{\partial u}{\partial x} + u \frac{\partial \rho}{\partial x} \\ u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} \\ \gamma p \frac{\partial u}{\partial x} + u \frac{\partial p}{\partial x} \end{pmatrix} = 0$$

primitive variables

- Define auxiliary variable: $q = 1/\rho$
- Take derivative: $\frac{\partial q}{\partial t} = \frac{-1}{\rho^2} \frac{\partial \rho}{\partial t} = \frac{-1}{\rho^2} \left(-\rho \frac{\partial u}{\partial x} - u \frac{\partial \rho}{\partial x} \right) = q \frac{\partial u}{\partial x} - u \frac{\partial q}{\partial x}$

$$\frac{\partial}{\partial t} \begin{pmatrix} u \\ p \\ q \end{pmatrix} + \begin{pmatrix} u \frac{\partial u}{\partial x} + q \frac{\partial p}{\partial x} \\ \gamma p \frac{\partial u}{\partial x} + u \frac{\partial p}{\partial x} \\ q \frac{\partial u}{\partial x} + u \frac{\partial q}{\partial x} \end{pmatrix} = 0$$

lifted variables



$$\mathbf{E}\dot{\mathbf{x}} = \underbrace{\mathbf{A}\mathbf{x} + \mathbf{B}u}_{\text{linear}} + \underbrace{\mathbf{H}(\mathbf{x} \otimes \mathbf{x})}_{\text{quadratic}}$$

lifted system

Lifting example: Tubular reactor

ψ : species concentration

θ : temperature

\mathcal{D} : Damköhler number

Pe : Péclet number

$\beta, B, \theta_0, \gamma$: known constants

Governing equations:

$$\dot{\psi} = \frac{1}{Pe} \psi_{ss} - \psi_s - \mathcal{D} \psi e^{\gamma - \frac{\gamma}{\theta}}, \quad s \in (0, 1), \quad t > 0$$

$$\dot{\theta} = \frac{1}{Pe} \theta_{ss} - \theta_s - \beta(\theta - \theta_{\text{ref}}) + \mathcal{B} \mathcal{D} \psi e^{\gamma - \frac{\gamma}{\theta}}$$

Lifting transformations: $w_1 = e^{\gamma - \frac{\gamma}{\theta}}, \quad w_2 = \theta^{-2}, \quad w_3 = \theta^{-1}$

Auxiliary dynamics for lifted variables are quartic:

$$\dot{w}_1 = w_1(\gamma - \theta^{-2})\dot{\theta} = \gamma \underbrace{w_1 w_2 \dot{\theta}}_{\text{quartic}}$$

$$\dot{w}_2 = -2\theta^{-3}\dot{\theta} = -2 \underbrace{w_2 w_3 \dot{\theta}}_{\text{quartic}}$$

$$\dot{w}_3 = -\theta^{-2}\dot{\theta} = - \underbrace{w_2 \dot{\theta}}_{\text{cubic}}$$

...while the original equations become quadratic

$$\dot{\psi} = \underbrace{\frac{1}{Pe} \psi_{ss} - \psi_s - \mathcal{D}}_{\text{linear}} \underbrace{\psi w_1}_{\text{quadratic}}$$

$$\dot{\theta} = \underbrace{\frac{1}{Pe} \theta_{ss} - \theta_s - \beta(\theta - \theta_{\text{ref}}) + \mathcal{B} \mathcal{D}}_{\text{linear}} \underbrace{\psi w_1}_{\text{quadratic}}$$

Lifting example: Tubular reactor

Quadratic-bilinear form
achievable with
differential-algebraic
equations (DAEs)

To get to QB form, need additional auxiliary variables:

$$w_4 = \psi w_1, \quad w_5 = w_2 w_3, \quad w_6 = w_1 w_2$$

The lifted system then becomes a quadratic-bilinear DAE:

$$\dot{\psi} = \underbrace{\frac{1}{Pe} \psi_{ss} - \psi_s - \mathcal{D} w_4}_{\text{linear}}$$

$$\dot{\theta} = \underbrace{\frac{1}{Pe} \theta_{ss} - \theta_s - \beta(\theta - \theta_{\text{ref}}) + \mathcal{B} \mathcal{D} w_4}_{\text{linear}}$$

$$\dot{w}_1 = \gamma w_6 \left[\frac{1}{Pe} \psi_{ss} - \psi_s \right] + \gamma \mathcal{B} \mathcal{D} w_4 w_6$$

$$\dot{w}_2 = -2 w_5 \left[\frac{1}{Pe} \psi_{ss} - \psi_s \right] - 2 \mathcal{B} \mathcal{D} w_4 w_5$$

$$\dot{w}_3 = -w_2 \left[\frac{1}{Pe} \psi_{ss} - \psi_s \right] - \mathcal{B} \mathcal{D} w_2 w_4$$

$$0 = w_4 - w_1 \psi$$

$$0 = w_5 - w_2 w_3$$

$$0 = w_6 - w_1 w_2$$

Lifting summary: Tubular reactor

- Introduce six auxiliary variables;
state increase from $2n$ to $8n$
- Lift to a QB-DAE

$$\mathbf{E}\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u} + \mathbf{H}(\mathbf{x} \otimes \mathbf{x}) + \sum_{k=1}^m \mathbf{N}_k \mathbf{x} u_k$$

lifted QB-DAE

$$\hat{\mathbf{E}}\dot{\hat{\mathbf{x}}} = \hat{\mathbf{A}}\hat{\mathbf{x}} + \hat{\mathbf{B}}\mathbf{u} + \hat{\mathbf{H}}(\hat{\mathbf{x}} \otimes \hat{\mathbf{x}}) + \sum_{k=1}^m \hat{\mathbf{N}}_k \hat{\mathbf{x}} u_k$$

QB ROM

$$\begin{aligned} \dot{\psi} &= \frac{1}{Pe} \psi_{ss} - \psi_s - \mathcal{D}\psi e^{\gamma - \frac{\gamma}{\theta}} \\ \dot{\theta} &= \frac{1}{Pe} \theta_{ss} - \theta_s - \beta(\theta - \theta_{\text{ref}}) + \mathcal{B}\mathcal{D}\psi e^{\gamma - \frac{\gamma}{\theta}} \end{aligned}$$

original equations

$$\begin{aligned} \dot{\psi} &= \underbrace{\frac{1}{Pe} \psi_{ss} - \psi_s - \mathcal{D}w_4}_{\text{linear}} \\ \dot{\theta} &= \underbrace{\frac{1}{Pe} \theta_{ss} - \theta_s - \beta(\theta - \theta_{\text{ref}}) + \mathcal{B}\mathcal{D}w_4}_{\text{linear}} \end{aligned}$$

$$\dot{w}_1 = \gamma w_6 \left[\frac{1}{Pe} \psi_{ss} - \psi_s \right] + \gamma \mathcal{B}\mathcal{D} w_4 w_6$$

$$\dot{w}_2 = -2 w_5 \odot \left[\frac{1}{Pe} \psi_{ss} - \psi_s \right] - 2\mathcal{B}\mathcal{D} w_4 w_5$$

$$\dot{w}_3 = -w_2 \odot \left[\frac{1}{Pe} \psi_{ss} - \psi_s \right] - \mathcal{B}\mathcal{D} w_2 w_4$$

$$0 = w_4 - w_1 \psi$$

$$0 = w_5 - w_2 w_3$$

$$0 = w_6 - w_1 w_2$$

lifted equations

Tubular reactor: QB-POD ROM

- Finite difference discretization with n points per unknown
- Recorded snapshots for POD every $\Delta t = 0.01s$

Original system

$$\dot{\mathbf{x}} = f(\mathbf{x}) + \mathbf{B}u$$

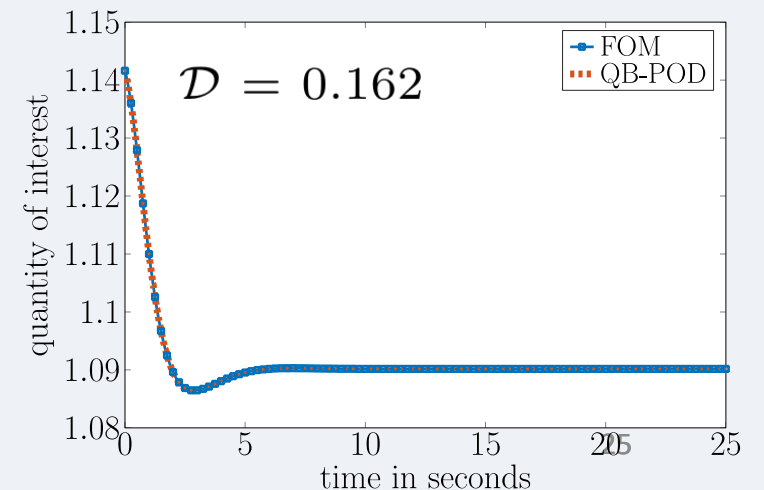
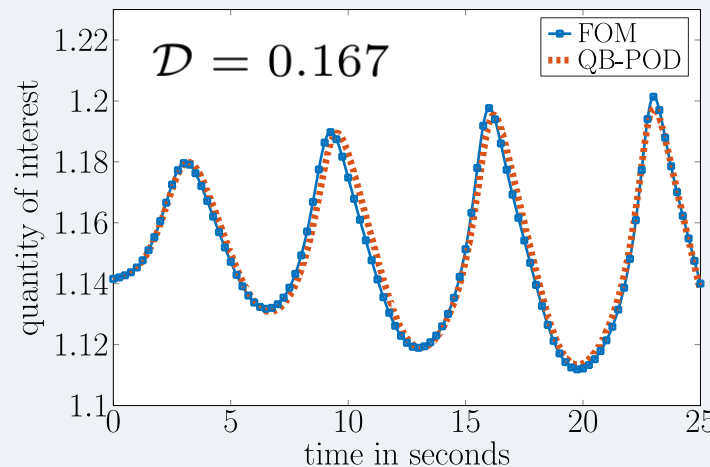
$$\begin{cases} \dot{\psi} = \mathbf{A}_\psi \psi + \mathbf{b}_\psi u(t) - \mathcal{D} \psi \odot e^{\gamma - \frac{\gamma}{\theta}} \\ \dot{\theta} = \mathbf{A}_\theta \theta + \mathbf{b}_\theta u(t) + \mathcal{B}\mathcal{D} \psi \odot e^{\gamma - \frac{\gamma}{\theta}} \end{cases}$$

Lifted system

$$\mathbf{E}\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}u + \mathbf{H}(\mathbf{x} \otimes \mathbf{x}) + \sum_{k=1}^m \mathbf{N}_k \mathbf{x} u_k$$

$$\begin{cases} \dot{\psi} = \mathbf{A}_\psi \psi + \mathbf{b}_\psi u(t) - \mathcal{D} \mathbf{w}_4 \\ \dot{\theta} = \mathbf{A}_\theta \theta + \mathbf{b}_\theta u(t) + \mathcal{B}\mathcal{D} \mathbf{w}_4 \\ \dot{\mathbf{w}}_1 = \gamma \mathbf{w}_6 \odot [A_2 \theta + \mathbf{b}_\theta u(t)] + \gamma \mathcal{B}\mathcal{D} \mathbf{w}_4 \odot \mathbf{w}_6 \\ \dot{\mathbf{w}}_2 = -2 \mathbf{w}_5 \odot [A_2 \theta + \mathbf{b}_\theta u(t)] - 2\mathcal{B}\mathcal{D} \mathbf{w}_4 \odot \mathbf{w}_5 \\ \dot{\mathbf{w}}_3 = -\mathbf{w}_2 \odot [A_2 \theta + \mathbf{b}_\theta u(t)] - \mathcal{B}\mathcal{D} \mathbf{w}_2 \odot \mathbf{w}_4 \\ 0 = \mathbf{w}_4 - \mathbf{w}_1 \odot \psi \\ 0 = \mathbf{w}_5 - \mathbf{w}_2 \odot \mathbf{w}_3 \\ 0 = \mathbf{w}_6 - \mathbf{w}_1 \odot \mathbf{w}_2 \end{cases}$$

QB-POD ROM: $\hat{\mathbf{E}}\dot{\hat{\mathbf{x}}} = \hat{\mathbf{A}}\hat{\mathbf{x}} + \hat{\mathbf{B}}u + \hat{\mathbf{H}}(\hat{\mathbf{x}} \otimes \hat{\mathbf{x}}) + \sum_{k=1}^m \hat{\mathbf{N}}_k \hat{\mathbf{x}} u_k$
 $r_1 = 30, r_2 = 9$



Summary

- Physics-based models have **structure**; learned models should exploit/respect that structure
- **Projection**: a structure-preserving lens

Learn

Infer a low-dimensional model directly from data of the original system, but through the lens of projection

Lift

Introduce transformations and auxiliary variables to express the physics in a structured form, then learn a reduced model

→ Elizabeth Qian talk, Tuesday 1035h (401A) & Thursday 1505h (401C)

Particularize

Use particular solutions to enforce boundary conditions and other physical constraints → Renee Swischuk poster, Tuesday PM

Data-driven decisions

building the mathematical foundations and computational methods to enable design of the next generation of engineered systems

— KIWI.ICES.UTEXAS.EDU —



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and Engineering Mechanics**
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