# Operator inference for non-polynomial systems & control applications<sup>1</sup>

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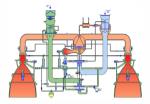
# Motivation: Learning ROMs for complex systems

#### Challenges in complex applications

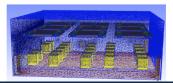
- Uncertainties in model, parameters, or both
- Details and access to governing equations, discretization, and solver typically unavailable when working with legacy codes ⇒ Intrusive MOR infeasible in those situations

### Opportunities

 Data is everywhere (cheaper memory, better sensors, more observations); can be used to build ROMs and/or reduce uncertainties







Dynamical systems nature of problem should not be ignored in model learning.

The more we know about the model, the more we can incorporate into the learning framework: Model structure, nonlinear terms, inputs, etc.

#### Partial Differential Equation Model

Many complex problems are modeled with PDEs of the form:

 $\frac{\partial s}{\partial t} = \mathcal{A}(s;q) + \mathcal{H}(s;q) + f(t,s;q) + \mathcal{B}(\mathbf{u};q)$ 

- $\blacksquare \ {\rm Input} \ {\bf u}(t)$
- State  $s(x,t;\mu)$  with  $x \in \Omega \subseteq \mathbf{R}^d, \ d = 1,2,3$
- Parameters q
- $\blacksquare \mathcal{A}$  is a linear operator
- $\mathcal{H}$  is quadratic in s, the nonlinear function is f(t,s) and  $\mathcal{B}$  is a linear input operator.

### Full-order model (FOM)

Semi-discretized numerical model of the PDE:

$$\begin{split} \dot{\mathbf{s}}(t,\mathbf{q}) = & \mathbf{A}(\mathbf{q})\mathbf{s}(t;\mathbf{q}) + \mathbf{H}(\mathbf{q})(\mathbf{s}(t;\mathbf{q}) \otimes \mathbf{s}(t;\mathbf{q})) \\ & + \mathbf{f}(t,\mathbf{s};\mathbf{q}) + \mathbf{B}(\mathbf{q})\mathbf{u}(t), \end{split}$$

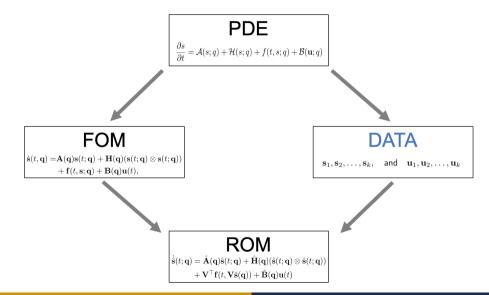
- State  $\mathbf{s}(t; \mathbf{q}) \in \mathbf{R}^n$
- Parameters  $\mathbf{q} \in \mathbf{R}^{\ell}$
- $\blacksquare$  Matrices  $\mathbf{A} \in \mathbf{R}^{n \times n}$ ,  $\mathbf{H} \in \mathbf{R}^{n \times n^2}$ ,  $\mathbf{B} \in \mathbf{R}^{n \times m}$

## Reduced-order model (ROM)

$$\begin{split} \dot{\hat{\mathbf{s}}}(t;\mathbf{q}) &= \hat{\mathbf{A}}(\mathbf{q})\hat{\mathbf{s}}(t;\mathbf{q}) + \hat{\mathbf{H}}(\mathbf{q})(\hat{\mathbf{s}}(t;\mathbf{q}) \otimes \hat{\mathbf{s}}(t;\mathbf{q})) \\ &+ \mathbf{V}^{\top}\mathbf{f}(t,\mathbf{V}\hat{\mathbf{s}}(\mathbf{q})) + \hat{\mathbf{B}}(\mathbf{q})\mathbf{u}(t) \end{split}$$

- $\blacksquare$  Reduced state  $\widehat{\mathbf{s}}(t;\mathbf{q})\in\mathbf{R}^n$
- $\blacksquare$  Parameters  $\mathbf{q} \in \mathbf{R}^\ell$
- Matrices  $\hat{\mathbf{A}} \in \mathbf{R}^{r \times r}$ ,  $\hat{\mathbf{H}} \in \mathbf{R}^{r \times r^2}$ ,  $\hat{\mathbf{B}} \in \mathbf{R}^{r \times m}$

## Intrusive vs. non-intrusive: Sometimes we don't have a choice



## Part 1:

## Operator Inference for non-intrusive model reduction of systems with non-polynomial nonlinear terms (hopefully completed soon)

with Peter Benner, Pawan Goyal, Benjamin Peherstorfer, Karen Willcox

## Part 1: Problem setting & Goal

1. Model is known in PDE form (quadratic + non-polynomial + input):

$$\frac{\partial s}{\partial t} = \mathcal{A}(s) + \mathcal{H}(s) + f(t,s) + \mathcal{B}(\mathbf{u})$$

2. Data available from FOM<sup>2</sup>:

$$\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_k,$$
 and  $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_k$ 

3. The non-polynomial nonlinear term is such that:

$$\mathbf{f}(t,\mathbf{s}) = [f(t,s_1), \cdots, f(t,s_n)]^{\top}$$

#### Goal

Leverage available information of nonlinear terms to learn a ROM:

$$\dot{\hat{\mathbf{s}}}(t) = \hat{\mathbf{A}}\hat{\mathbf{s}}(t) + \hat{\mathbf{H}}(\hat{\mathbf{s}}(t) \otimes' \hat{\mathbf{s}}(t)) + \mathbf{V}^{\top}\mathbf{f}(t, \mathbf{V}\hat{\mathbf{s}}) + \hat{\mathbf{B}}\mathbf{u}(t)$$

<sup>2</sup>The FOM data comes from time-stepping  $\dot{\mathbf{s}}(t) = \mathbf{As}(t) + \mathbf{H}(\mathbf{s}(t) \otimes' \mathbf{s}(t)) + \mathbf{f}(t, \mathbf{s}) + \mathbf{Bu}(t)$ 

## A short example

## Consider the PDE

$$\frac{\partial}{\partial t}s(x,t) = \frac{\partial^2}{\partial x^2}s(x,t) + e^{-\beta t}s(x,t)^{-\alpha} + b(x)u(t)$$

with time-dependent reaction term  $f(t,s) = e^{-\beta t}s(x,t)^{-\alpha}$ . After spatial discretization with a finite difference scheme, the system reads as  $(\mathbf{s}^{-\alpha} := [s_i]^{-\alpha}, \ i = 1, 2, \dots, n)$ :

$$\dot{\mathbf{s}}(t) = \mathbf{A}\mathbf{s}(t) + e^{-\beta t}\mathbf{s}(t)^{-\alpha} + \mathbf{B}u(t).$$

**f** $(t, \mathbf{s}(t)) = e^{-\beta t} \mathbf{s}(t)^{-\alpha}$  does not require approximation of spatial derivatives

Evaluating the semi-discrete nonlinear function f(t, s) only requires application of  $f(t, s_i)$  at every component of  $s = [s_1, s_2, \dots, s_n]$ .

**Other examples**: Arrhenius reaction model  $\exp(\gamma - \frac{\gamma}{s})$ ; rational functions  $\frac{s}{\alpha + s}$ , fractional powers  $s^{\alpha}$  etc.

## Intrusive projection-based ROMs

Given is the following FOM, and we would like to compute a ROM:

 $\dot{\mathbf{s}}(t) = \mathbf{A}\mathbf{s}(t) + \mathbf{H}(\mathbf{s}(t) \otimes' \mathbf{s}(t)) + \mathbf{f}(t, \mathbf{s}) + \mathbf{B}\mathbf{u}(t)$ 

•  $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_r] \in \mathbf{R}^{n \times r}$  orthonormal matrix,  $r \ll n$ , computed, e.g., with POD.

• Let  $ilde{\mathbf{s}}$  be the ROM state with  $\mathbf{s}_i pprox \mathbf{V} ilde{\mathbf{s}}_i$ 

#### Projection-based (intrusive) ROM

The projection-based ROM has the form

$$\dot{\widetilde{\mathbf{s}}}(t) = \widetilde{\mathbf{A}}\widetilde{\mathbf{s}}(t) + \widetilde{\mathbf{H}}(\widetilde{\mathbf{s}}(t) \otimes' \widetilde{\mathbf{s}}(t)) + \widetilde{\mathbf{f}}(t,\widetilde{\mathbf{s}}) + \widetilde{\mathbf{B}}\mathbf{u}(t)$$

where  $\ \widetilde{\mathbf{f}}(t,\widetilde{\mathbf{s}}) = \mathbf{V}^{\top}\mathbf{f}(t,\mathbf{V}\widetilde{\mathbf{s}})$  and the reduced operators

$$\widetilde{\mathbf{A}} = \mathbf{V}^\top \mathbf{A} \mathbf{V} \in \mathbf{R}^{r \times r} \,, \quad \widetilde{\mathbf{H}} = \mathbf{V}^\top \mathbf{H} (\mathbf{V} \otimes' \mathbf{V}) \in \mathbf{R}^{r \times r^2} \,, \quad \widetilde{\mathbf{B}} = \mathbf{V}^\top \mathbf{B} \in \mathbf{R}^{r \times m}$$

# Non-intrusive Operator Inference: Preparing the data

To learn a ROM, we build on the operator inference work from [Peherstorfer and Willcox, 2016]:

1. Start with state and input data:

$$\mathbf{S} := \begin{bmatrix} | & | & \dots & | \\ \mathbf{s}_0 & \mathbf{s}_1 & \dots & \mathbf{s}_k \\ | & | & \dots & | \end{bmatrix}, \qquad \mathbf{U} := \begin{bmatrix} | & | & | & \dots & | \\ \mathbf{u}(t_0) & \mathbf{u}(t_1) & \dots & \mathbf{u}(t_k) \\ | & | & | & | \end{bmatrix}.$$

2. Due to the specific form of the nonlinear terms, we can evaluate the nonlinear snapshot matrix:

$$\mathbf{F} = \begin{bmatrix} | & | & | \\ \mathbf{f}(t_0, \mathbf{s}(t_0)) & \mathbf{f}(t_1, \mathbf{s}(t_1)) & \cdots & \mathbf{f}(t_k, \mathbf{s}(t_k)) \\ | & | & | & | \end{bmatrix}.$$

3. Compute r dominant POD basis vectors of S, resulting in V s.t.  $\|S\|$ 

$$\frac{-\mathbf{V}\mathbf{V}^{\top}\mathbf{S}\|}{\|\mathbf{S}\|} \leq \texttt{tol}$$

4. Project the state data and nolinear snapshot data

$$\hat{\mathbf{S}} = \mathbf{V}^{\top} \mathbf{S}, \qquad \hat{\mathbf{F}} = \mathbf{V}^{\top} \mathbf{F}.$$

# **Operator inference: Solving for the operators**

Denote with  $\hat{\mathbf{s}}_k$  the time derivative approximation of  $\frac{d}{dt}\hat{\mathbf{s}}(t_k)$ , which can be computed from  $\hat{\mathbf{s}}$  using a time derivative approximation. We store the time-derivative approximations in the matrix

$$\dot{\widehat{\mathbf{S}}} := \begin{bmatrix} \begin{vmatrix} & & & & \\ \hat{\mathbf{s}}(t_0) & \hat{\mathbf{s}}(t_1) & \cdots & \hat{\mathbf{s}}(t_k) \\ & & & & \end{vmatrix}.$$

Operator inference for non-polynomial nonlinear system

A non-intrusive ROM of the form

$$\dot{\hat{\mathbf{s}}}(t) = \hat{\mathbf{A}}\hat{\mathbf{s}}(t) + \hat{\mathbf{H}}(\hat{\mathbf{s}}(t) \otimes' \hat{\mathbf{s}}(t)) + \mathbf{V}^{\top}\mathbf{f}(t, \mathbf{V}\hat{\mathbf{s}}(t)) + \hat{\mathbf{B}}\mathbf{u}(t),$$

can be obtained by solving the optimization problem from the above projected:

$$\min_{\hat{\mathbf{A}},\hat{\mathbf{B}},\hat{\mathbf{H}}} \| \underbrace{\dot{\hat{\mathbf{S}}} - \hat{\mathbf{F}}}_{:=\hat{\mathbf{R}}} - \hat{\mathbf{A}}\hat{\mathbf{S}} - \hat{\mathbf{B}}\mathbf{U} - \hat{\mathbf{H}}(\hat{\mathbf{S}}\otimes'\hat{\mathbf{S}}) \|_F.$$

#### **Assumption 1**

The time stepping scheme for the FOM is convergent, i.e.,

$$\max_{i \in \{1, \dots T/\Delta t\}} \|\mathbf{s}_i - \mathbf{s}(t_i)\|_2 \to 0 \quad \text{as} \quad \Delta t \to 0.$$

#### **Assumption 2**

The derivatives approximated from projected states,  $\dot{\hat{s}}_k$ , converge to  $\frac{d}{dt}\hat{s}(t_k)$  as the discretization time step  $\Delta t \rightarrow 0$ , i.e.,

$$\max_{i \in \{1, \dots, T/\Delta t\}} \|\dot{\hat{\mathbf{s}}}_i - \frac{\mathsf{d}}{\mathsf{d}t} \hat{\mathbf{s}}(t_i)\|_2 \to 0 \quad \text{as} \quad \Delta t \to 0.$$

#### Theorem [Benner/Goyal/K./Peherstorfer/Willcox, 2020]

Let Assumption 1 and Assumption 2 hold and let a POD basis matrix  $\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_r] \in \mathbf{R}^{n \times r}$  be given. Let  $\widetilde{\mathbf{A}}, \widetilde{\mathbf{B}}, \widetilde{\mathbf{H}}$  be the intrusively projected ROM operators. Let the data matrix  $[\hat{\mathbf{S}}, \mathbf{U}, \hat{\mathbf{S}} \otimes' \hat{\mathbf{S}}]$  have full column rank.

Then for every  $\varepsilon > 0$ , there exists  $r \le n$  and a time step size  $\Delta t > 0$  such that the learned operators satisfy:

$$\|\hat{\mathbf{A}} - \widetilde{\mathbf{A}}\| \le \varepsilon, \qquad \|\hat{\mathbf{B}} - \widetilde{\mathbf{B}}\| \le \varepsilon, \qquad \|\hat{\mathbf{H}} - \widetilde{\mathbf{H}}\| \le \varepsilon.$$

To accelerate the evaluation of  $\mathbf{V}^{\top}\mathbf{f}(t, \mathbf{V}\hat{\mathbf{s}})$  in the learned ROM, hyper-reduction can be used (Barrault et al., 2004; Astrid et al., 2008; Nguyen et al., 2008, Chaturantabut & Sorensen, 2010; Carlberg et al., 2013; Drmac & Gugercin, 2016,...)

We employ the discrete empirical interpolation method (DEIM) to approximate

$$\hat{\mathbf{f}}(t, \mathbf{V}\hat{\mathbf{s}}) \approx \hat{\mathbf{f}}_r(t, \mathbf{V}\hat{\mathbf{s}}) = \mathbf{V}^\top \mathbf{W}(\mathbb{S}^\top \mathbf{W})^{-1} \mathbb{S}^\top \mathbf{f}(t, \mathbf{V}\hat{\mathbf{s}}).$$

- W is computed by taking the SVD of the nonlinear snapshot matrix F and setting W to the leading *m* left singular vectors of F.
- S is an  $n \times m$  matrix obtained by selecting certain columns of the  $n \times n$  identity matrix, following the DEIM algorithm.

## **Results: Tubular reactor model**

One-dimensional ( $x \in (0,1)$ ) model with a single reaction, describing the evolution of the species concentration  $\psi(x,t)$  and temperature  $\theta(x,t)$  via

$$\begin{aligned} \frac{\partial \psi}{\partial t} &= \frac{1}{\text{Pe}} \frac{\partial^2 \psi}{\partial x^2} - \frac{\partial \psi}{\partial x} - \mathcal{D}f(\psi,\theta;\gamma),\\ \frac{\partial \theta}{\partial t} &= \frac{1}{\text{Pe}} \frac{\partial^2 \theta}{\partial x^2} - \frac{\partial \theta}{\partial x} - \beta(\theta - \theta_{\text{ref}}) + \mathcal{B}\mathcal{D}f(\psi,\theta;\gamma), \end{aligned}$$

with Arrhenius reaction term

$$f(\psi, \theta; \gamma) = \psi \exp\left(\gamma - \frac{\gamma}{\theta}\right).$$

Boundary conditions

$$\frac{\partial \psi}{\partial x}(0,t) = \operatorname{Pe}(\psi(0,t)-1), \quad \frac{\partial \theta}{\partial x}(0,t) = \operatorname{Pe}(\theta(0,t)-1), \quad \frac{\partial \psi}{\partial x}(1,t) = 0, \quad \frac{\partial \theta}{\partial x}(1,t) = 0.$$

The quantity of interest is the temperature oscillation at the reactor exit:

$$y(t) = \theta(x = 1, t).$$

## **Results: Tubular reactor model**

■ FOM is semi-discrete model obtained via finite differences:

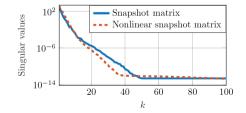
$$\dot{\mathbf{s}}(t) = \mathbf{A}\mathbf{s}(t) + \mathbf{f}(\mathbf{s}(t)) + \mathbf{B}.$$

with discretized state  $\mathbf{s}(t) \in \mathbb{R}^{198}$ .

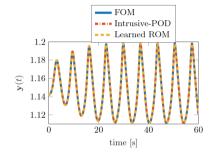
Discretized Arrhenius term requires pointwise evaluations (local in space)

$$[\mathbf{f}(\boldsymbol{\psi}, \boldsymbol{\theta}; \gamma)]_i = \psi_i \exp\left(\gamma - \frac{\gamma}{\theta_i}\right).$$

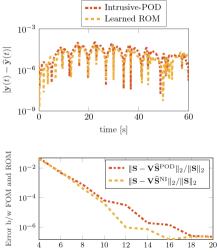
• Collect snapshots in T = (0, 30] with  $\delta t = 10^{-3}$  spacing.



# Learned ROM more accurate than intrusive ROM



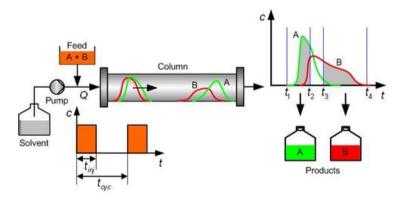
- ROM predictions for 100% longer than training interval
- $\blacksquare \ r=10$  for both ROMs
- Learned ROM (non-Markovian) more accurate than projection-based ROM



reduced model dimension

# Batch Chromatography: A chemical process

- Mixture of products A and B injected into column
- Move with different velocities, thus separating at the column exit
- Component A, which moves faster, is collected between  $t_1$  and  $t_2$ , component B between  $t_3$  and  $t_4$



# Batch Chromatography: A non-polynomial nonlinear model

The dynamics of the batch chromatographic column:

$$\frac{\partial c_i}{\partial t} + \frac{1-\epsilon}{\epsilon} \frac{\partial q_i}{\partial t} + \nu \frac{\partial c_i}{\partial x} - D_i \frac{\partial^2 c_i}{\partial x^2} = 0$$
$$\frac{\partial q_i}{\partial t} = \kappa_i \left( q_i^{Eq} - q_i \right)$$

Adsorption equilibrium concentration

$$q_i^{\mathsf{Eq}} = \frac{H_{i,1} \, c_i}{1 + \sum_{j=1,2} K_{j,1} \, c_j} + \frac{H_{i,2} \, c_i}{1 + \sum_{j=1,2} K_{j,2} \, c_j}$$

- $c_i, q_i$ : Liquid & solid phase concentration
- $H_{i,1}, H_{i,2}$ : Henry constants
- $K_{j,1}, K_{j,2}$  the thermodynamic coefficients
- $\kappa_i$ : mass-transfer coefficient of component i
- $\epsilon$ : column porosity

- Zero initial conditions  $c_i(t = 0, x) = q_i(t = 0, x) = 0$
- Boundary conditions:

$$D_i \left. \frac{\partial c_i}{\partial x} \right|_{x=0} = \nu \left( \left. c_i \right|_{x=0} - c_i^{\text{in}} \right), \quad \left. \frac{\partial c_i}{\partial x} \right|_{x=L} = 0$$

with

$$c_i^{\rm in}(t) = \frac{1}{1 + e^{-5(t - t_{\rm inj})}}, \quad t_{\rm inj} = 1.3$$

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## Creating a block-structured model

We can simplify the previous PDE by inserting  $\dot{q}_i$  into the first equation, and obtain:

$$\begin{split} \frac{\partial c_i}{\partial t} &= -\nu \frac{\partial c_i}{\partial x} + D_i \frac{\partial^2 c_i}{\partial x^2} + \epsilon_c \kappa_i \left( q_i^{Eq} - q_i \right) \\ \frac{\partial q_i}{\partial t} &= \kappa_i \left( q_i^{Eq} - q_i \right) \end{split}$$

A finite volume discretization of the governing equations yields a discretized model of the form:

$$\begin{bmatrix} \dot{\mathbf{c}}_1 \\ \dot{\mathbf{q}}_1 \\ \dot{\mathbf{c}}_2 \\ \dot{\mathbf{q}}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{A}_1 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{0} & 0 \\ 0 & 0 & \mathbf{A}_2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{q}_1 \\ \mathbf{c}_2 \\ \mathbf{q}_2 \end{bmatrix} + \begin{bmatrix} \mathbf{B} \\ 0 \\ \mathbf{B} \\ 0 \end{bmatrix} u(t) + \begin{bmatrix} \epsilon_c \\ 1 \end{bmatrix} \otimes \begin{bmatrix} \mathbf{f}_1(\mathbf{c}_1, \mathbf{q}_1, \mathbf{c}_2, \mathbf{q}_2) \\ \mathbf{f}_2(\mathbf{c}_1, \mathbf{q}_1, \mathbf{c}_2, \mathbf{q}_2) \end{bmatrix},$$

where  $c_1, q_1, c_2, q_2 \in \mathbf{R}^n$ ,  $A_1, A_2 \in \mathbf{R}^{n \times n}$ ,  $\mathbf{B} \in \mathbf{R}^n$ . The nonlinear term is spatially local

$$\mathbf{f}_i(\mathbf{c}_1, \mathbf{q}_1, \mathbf{c}_2, \mathbf{q}_2) = \kappa_i \left( \mathbf{q}_i^{\mathsf{Eq}} - \mathbf{q}_i 
ight)$$

# Maintaining the coupling structure in projection-based ROMs

In a projection-based framework, we would approximate

$$\begin{bmatrix} \mathbf{c}_1 \\ \mathbf{q}_1 \\ \mathbf{c}_2 \\ \mathbf{q}_2 \end{bmatrix} \approx \begin{bmatrix} \mathbf{V}_{\mathbf{c}_1} & & & \\ & \mathbf{V}_{\mathbf{q}_1} & & \\ & & \mathbf{V}_{\mathbf{c}_2} & \\ & & & \mathbf{V}_{\mathbf{q}_2} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{c}}_1 \\ \hat{\mathbf{q}}_1 \\ \hat{\mathbf{c}}_2 \\ \hat{\mathbf{q}}_2 \end{bmatrix}$$

so that the ROM preserves the coupling structure:

$$\begin{bmatrix} \dot{\hat{\mathbf{c}}}_1 \\ \dot{\hat{\mathbf{q}}}_1 \\ \dot{\hat{\mathbf{c}}}_2 \\ \dot{\hat{\mathbf{q}}}_2 \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{A}}_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \hat{\mathbf{A}}_2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \hat{\mathbf{c}}_1 \\ \hat{\mathbf{q}}_1 \\ \hat{\mathbf{c}}_2 \\ \hat{\mathbf{q}}_2 \end{bmatrix} + \begin{bmatrix} \hat{\mathbf{B}}_1 \\ 0 \\ \hat{\mathbf{B}}_2 \\ 0 \end{bmatrix} u(t) + \begin{bmatrix} \epsilon_c \\ 1 \end{bmatrix} \otimes \begin{bmatrix} \hat{\mathbf{f}}_1(\hat{\mathbf{c}}_1, \hat{\mathbf{q}}_1, \hat{\mathbf{c}}_2, \hat{\mathbf{q}}_2) \\ \hat{\mathbf{f}}_2(\hat{\mathbf{c}}_1, \hat{\mathbf{q}}_1, \hat{\mathbf{c}}_2, \hat{\mathbf{q}}_2) \end{bmatrix},$$

where  $\hat{\mathbf{c}}_1, \hat{\mathbf{q}}_1, \hat{\mathbf{c}}_2, \hat{\mathbf{q}}_2 \in \mathbf{R}^r$ ,  $\hat{\mathbf{A}}_1, \hat{\mathbf{A}}_2 \in \mathbf{R}^{r \times r}$ ,  $\hat{\mathbf{B}}_1, \hat{\mathbf{B}}_2 \in \mathbf{R}^r$ .

# Using our model knowledge: Maintaining the coupling structure in learned ROMs

For Operator Inference, we assemble the following data (with T = (0, 10]s and  $\delta t = 10^{-5}$ ):

$$\hat{\mathbf{S}} = \begin{bmatrix} \mathbf{V}_{\mathbf{c}_1}^\top \mathbf{C}_1 \\ \mathbf{V}_{\mathbf{q}_1}^\top \mathbf{Q}_1 \\ \mathbf{V}_{\mathbf{c}_2}^\top \mathbf{C}_2 \\ \mathbf{V}_{\mathbf{q}_2}^\top \mathbf{Q}_2 \end{bmatrix} =: \begin{bmatrix} \hat{\mathbf{C}}_1 \\ \hat{\mathbf{Q}}_1 \\ \hat{\mathbf{C}}_2 \\ \hat{\mathbf{Q}}_2 \end{bmatrix}, \qquad \hat{\mathbf{S}} = \begin{bmatrix} \mathbf{V}_{\mathbf{c}_1}^\top \dot{\mathbf{C}}_1 \\ \mathbf{V}_{\mathbf{q}_1}^\top \dot{\mathbf{Q}}_1 \\ \mathbf{V}_{\mathbf{c}_2}^\top \dot{\mathbf{C}}_2 \\ \mathbf{V}_{\mathbf{q}_2}^\top \dot{\mathbf{Q}}_2 \end{bmatrix} =: \begin{bmatrix} \hat{\mathbf{C}}_1 \\ \hat{\mathbf{Q}}_1 \\ \hat{\mathbf{C}}_2 \\ \hat{\mathbf{Q}}_2 \end{bmatrix}$$

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Block structure preservation in learned ROM

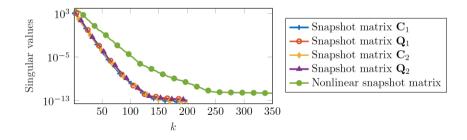
We can maintain the coupling structure by **solving separate least-squares problems** of the form

$$\min_{\hat{\mathbf{A}}_i, \hat{\mathbf{B}}_i} \| \hat{\mathbf{C}}_i - \epsilon_c \mathbf{V}_{\mathbf{c}_i}^\top \mathbf{F} - \hat{\mathbf{A}}_i \hat{\mathbf{C}}_i - \hat{\mathbf{B}}_i \mathbf{U} \|_F, \quad i \in \{1, 2\}.$$

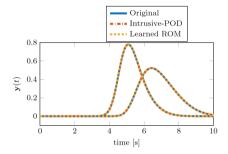
- Important for physical interpretability of the model
- Numerical implications, stability [Liao et al., 2007; Reis & Stykel, 2007, 2008; Benner & Feng, 2015; Kramer, 2016]

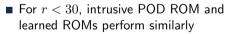
## Learned ROM and projection-based ROM

- Both the learned ROM and intrusive ROM retain coupling structure
- Singular values decay rather slowly due to transport nature of Batch Chromatography
- **ROMs** of order r = 22 for each variable
- **DEIM** approximation used for nonlinear term  $\mathbf{f}_i(\mathbf{c}_1, \mathbf{q}_1, \mathbf{c}_2, \mathbf{q}_2)$

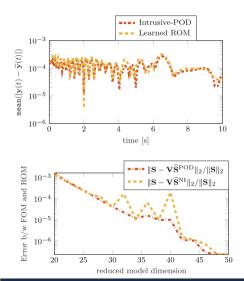


# Learned ROM accuracy





■ For r > 30 the learned ROM does not converge monotonely ⇒ Condition number of Operator Inference problem, or closure issue (Re-projection?).



# Conclusions: Learned ROMs with non-polynomial structure

Accurate non-intrusive ROMs possible with Operator Inference learning framework

- Convergence results shows that under mild assumptions on the time stepping and step size, the non-intrusively learned reduced models converge to the same reduced models as obtained with intrusive model reduction methods.
- The more we know about the model, the more we can incorporate into the learning framework: Model structure, nonlinear terms, etc.

*Operator Inference for non-intrusive model reduction of systems with non-polynomial nonlinear terms*, Benner/Goyal/K./Peherstorfer/Willcox, 2020

## Part 2:

## Operator Inference to learn ROMs for control applications

*Feedback control for systems with uncertain parameters using online-adaptive reduced models.* K./Peherstorfer/Willcox, SIAM J. on Applied Dynamical Systems 16(3), pp. 1563-1586, 2017.

## Part 2: Problem setting & Goal

**Goal:** Control a plant that has the form:

 $\dot{\mathbf{s}}(t) = \mathbf{A}(\mathbf{q}(t))\mathbf{s}(t) + \mathbf{B}\mathbf{u}(t), \quad \mathbf{s}(0) = \mathbf{s}_0 \in \mathbb{R}^n$ 

with time-dependent parameters that assume a residence time:

$$\mathbf{q}(t) = \mathbf{q}_{\mathcal{T}_i}$$
 for  $t \in \mathcal{T}_i = [t_{i-1}, t_i]$ .

#### Problem setting and challenges:

- **Switching times**  $t_i$  not known a priori; have to be detected online
- **Dynamical system response changes with**  $\mathbf{q}(t)$  (stability, equilibria)
- Large-scale setting, (*n* large)
- Cannot evaluate  $\mathbf{A}(\mathbf{q}(t))$  online (b/c recourse to full model solver)

**Opportunities:** 

- State-space data from plant available
- Can use operator inference to learn ROM state-space model

## Formulating the control problem

Linear Quadratic Regulator Problem

$$\begin{split} \min_{\mathbf{u}} \quad J(\mathbf{s}, \mathbf{u}; \mathbf{q}) &= \int_0^\infty ||\mathbf{C}\mathbf{s}(t; \mathbf{q})||_2^2 + ||\mathbf{R}\mathbf{u}(t; q)||_2^2 \, \mathrm{d}t \\ \mathrm{s.t.} \quad \dot{\mathbf{s}}(t) &= \mathbf{A}(\mathbf{q}(t))\mathbf{s}(t) + \mathbf{B}\mathbf{u}(t), \quad \mathbf{s}(0) = \mathbf{s}_0 \ \in \mathbb{R}^n \end{split}$$

 $\mathbf{u}(t;q)$ : control;  $\mathbf{B}, \mathbf{C}$  known input and sensing matrices.

#### Control problem for plant with uncertainties

Let  $\mathbf{A}(\mathbf{q}(t))$  be available offline, but not online. Let  $\mathbf{B}, \mathbf{C}$  be available online. For all  $\mathcal{T}_i = [t_{i-1}, t_i], i = 1, 2, \dots$ , solve the control problem:

$$\begin{split} \min_{\mathbf{s}_{\mathcal{T}_i}, \mathbf{u}_{\mathcal{T}_i}} J(\mathbf{s}_{\mathcal{T}_i}, \mathbf{u}_{\mathcal{T}_i}) \\ \text{s.t.} \quad \dot{\mathbf{s}}_{\mathcal{T}_i}(t) = \mathbf{A}(\mathbf{q}_{\mathcal{T}_i}) \mathbf{s}_{\mathcal{T}_i}(t) + \mathbf{B} \mathbf{u}_{\mathcal{T}_i}(t) \end{split}$$

where the subscripts indicate the state and control in  $T_i = [t_{i-1}, t_i]$ .

### How can we detect switching $t_i$ ? How to deal with not-available $A(q_{T_i})$

#### Approach:

- Reduce-then-design approach: Design a controller based-on low-dimensional ROM
- $\blacksquare$  Use data to learn and update ROM matrix online  $\Rightarrow$  robustness to parametric changes

#### Algorithmic details:

- Offline: Library of high-fidelity solutions (subspaces, feedback gains)
- Online:
  - 1. Detect parameter-dependent subspace  $\mathbf{V} = \mathbf{V}(\mathbf{q}) \Rightarrow$  Deals with unknown switching times  $t_i$
  - 2. Learn system matrix  $\hat{\mathbf{A}}(\mathbf{q}(t)) = \mathbf{V}^{\top} \mathbf{A}(\mathbf{q}(t)) \mathbf{V}$  in real-time through data-driven ROMs; recompute optimal feedback from surrogate model

# **Related work**

#### Reduced-order modeling for control design:

[Burns and King, 1998, Burns et al., 1999, Kunisch and Volkwein, 1999, Atwell et al., 2001, Banks et al., 2000, Banks et al., 2002, Benner, 2004, Lee and Tran, 2005, Borggaard and Stoyanov, 2008, Sachs and Volkwein, 2010, Alla and Falcone, 2013, Nicaise et al., 2014, Tissot et al., 2015, Pyta et al., 2015] ..... Online-Interpolated ROMs for parameter-dependent systems

[Poussot-Vassal and Sipp, 2015]:

 ROMs generated offline for linearized equations; online interpolation (parameter known)

## Gain Scheduling for LPV systems

[Becker and Packard, 1994, Theis et al., 2016]

Linearization of NL systems around operating conditions/equlibria

# Offline (high fidelity)-online (compressed sensing detection) strategy [Mathelin et al., 2012]

• Controllers parametrized by initial condition

## Statistical learning strategy [Guéniat et al., 2016]

 Markov process model + Reinforcement learning for control law

# Learning LQR controller from random control input excitations [Dean et al., 2019, Cohen et al., 2019]

- Complete theory for error in learning unknown linear model  $(||\mathbf{A} \mathbf{A}^{est}|| < ..., ||\mathbf{B} \mathbf{B}^{est}|| < ... )$  and robust controller
- Finite-data results, but assumes randomized controller trials can be made

We approximate the dynamics as

$$\mathbf{s}(t;\mathbf{q}) \approx \mathbf{V}(\mathbf{q}) \hat{\mathbf{s}}(t;\mathbf{q}), \qquad \mathbf{V}(\mathbf{q}) \in \mathbb{R}^{n \times r}, \ r \ll n,$$

where  $\mathbf{V}(\mathbf{q})$  contains basis vectors for a low-dimensional, accurate representation of the dynamics. Enforcing orthogonality of the residual yields a ROM of similar structure

$$\dot{\hat{\mathbf{s}}}(t;\mathbf{q}) = \hat{\mathbf{A}}(\mathbf{q}(t))\hat{\mathbf{s}}(t;\mathbf{q}) + \hat{\mathbf{B}}\mathbf{u}(t),$$

where

$$\hat{\mathbf{A}}(\mathbf{q}) = \mathbf{V}(\mathbf{q})^{\top} \mathbf{A}(\mathbf{q}) \mathbf{V}(\mathbf{q}), \qquad \hat{\mathbf{B}}(\mathbf{q}) = \mathbf{V}(\mathbf{q})^{\top} \mathbf{B}.$$

We compute a library of subspaces V(q) for a suitably chosen selection  $\{q_1, q_2, \ldots, q_M\}$ .

# Low-rank structure in LQR

If  $(\mathbf{A}(\mathbf{q}),\mathbf{B})$  is stabilizable, then control assumes linear state feedback:

$$\mathbf{u}(t;q) = -\mathbf{K}(\mathbf{q})\mathbf{s}(t;\mathbf{q}) = -[\mathbf{R}^{-1}\mathbf{B}^{\top}\Pi(\mathbf{q})]\mathbf{s}(t;\mathbf{q}),$$
(2)

$$\mathbf{0} = \mathbf{A}^{\top}(\mathbf{q})\Pi(\mathbf{q}) + \Pi(\mathbf{q})\mathbf{A}(\mathbf{q}) - \Pi(\mathbf{q})\mathbf{B}\mathbf{B}^{\top}\Pi(\mathbf{q}) + \mathbf{C}^{\top}\mathbf{C}$$
(3)

where  $\mathbf{K}(\mathbf{q})$  is the gain matrix.

#### $\Pi(\mathbf{q})$ often of low numerical rank:

$$\Pi(\mathbf{q}) = \mathbf{W}(\mathbf{q})\mathbf{W}(\mathbf{q})^{\top}, \quad \mathbf{W}(\mathbf{q}) \in \mathbb{R}^{n \times r}$$

 $\Rightarrow$  Work with low-dimensional operators through  $\mathbf{V} \in \mathbb{R}^{n imes r}$ :

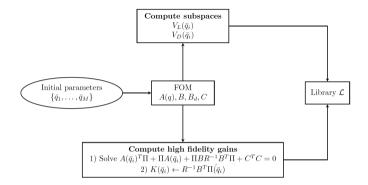
$$\hat{\mathbf{A}}(\mathbf{q}) = \mathbf{V}^{\top} \mathbf{A}(\mathbf{q}) \mathbf{V}, \quad \hat{\mathbf{B}} = \mathbf{V}^{\top} \mathbf{B}, \quad \hat{\mathbf{C}} = \mathbf{C} \mathbf{V}$$

Solve (3) in low dimensions (*reduce-then-design*):

$$\mathbf{0} = \hat{\mathbf{A}}^{\top}(\mathbf{q})\hat{\Pi}(\mathbf{q}) + \hat{\Pi}(\mathbf{q})\hat{\mathbf{A}}(\mathbf{q}) - \hat{\Pi}(\mathbf{q})\hat{\mathbf{B}}\hat{\mathbf{B}}^{\top}\hat{\Pi}(\mathbf{q}) + \hat{\mathbf{C}}^{\top}\hat{\mathbf{C}}$$

[Jbilou, 2003, Jbilou, 2006, Heyouni and Jbilou, 2009, Benner et al., 2008a, Benner et al., 2008b, Simoncini et al., 2013, Lin and Simoncini, 2014, Wang et al., 2014, Li et al., 2013, Kramer and Singler, 2016]...

# Offline: Pre-computing library of feedback gains



Feedback gains  $\mathbf{K}(\mathbf{q}_i)$ , learning bases  $\mathbf{V}_L(\mathbf{q}_i)$ , detection bases  $\mathbf{V}_D(\mathbf{q}_i)$ , for  $i = 1, \dots, M$ :

$$\mathcal{L} := \left\{ \left\{ \begin{matrix} \mathbf{V}_L(\mathbf{q}_1) \\ \mathbf{V}_D(\mathbf{q}_1) \\ \mathbf{K}(\mathbf{q}_1) \end{matrix} \right\}, \dots, \left\{ \begin{matrix} \mathbf{V}_L(\mathbf{q}_M) \\ \mathbf{V}_D(\mathbf{q}_M) \\ \mathbf{K}(q_M) \end{matrix} \right\} \right\}$$

# Online: Solving the classification problem

- S: selection operator that selects p' entries from the states  $\mathbf{s}(t;\mathbf{q}(t))$  with  $p' \in \{1,\ldots,n\}$  and  $p' \ll n$
- Detection subspaces  $\mathbf{V}_D(\bar{\mathbf{q}}_i), i = 1, \dots, M$
- $\blacksquare$  Define classifier  $h: \mathbb{R}^{p'} \to \{1, \dots, M\}$  via

 $h(\mathcal{S}\mathbf{s}(t; \bar{\mathbf{q}}_k)) = k$ 

• Solve classification problem by projection  $\mathbf{P}_i: \mathbb{R}^{p'} \mapsto \mathbb{R}^{p'}$ :

$$\mathbf{P}_{i} = \mathcal{S}\mathbf{V}_{D}(\bar{\mathbf{q}}_{i}) \left[ (\mathcal{S}\mathbf{V}_{D}(\bar{\mathbf{q}}_{i}))^{\top} (\mathcal{S}\mathbf{V}_{D}(\bar{\mathbf{q}}_{i})) \right]^{-1} (\mathcal{S}\mathbf{V}_{D}(\bar{\mathbf{q}}_{i}))^{\top}$$

Selected subspace:

$$k = \arg \max_{i=1,\dots,M} ||\mathbf{P}_i(\mathcal{S}\mathbf{s}(t;\mathbf{q}))||_2$$

Next step: Act on information and initiate model learning

# Online: ROM learning from recorded data

**Goal:** Learn ROM system matrix  $\hat{\mathbf{A}} = \hat{\mathbf{A}}(\tilde{\mathbf{q}}) \in \mathbb{R}^{r \times r}$  from data  $\mathbf{s}_1(\tilde{\mathbf{q}}), \dots, \mathbf{s}_\ell(\tilde{\mathbf{q}})$  and selected subspace  $\mathbf{V} = \mathbf{V}_L(\bar{\mathbf{q}}_k) \in \mathcal{L}$ .

- Compute  $\hat{\mathbf{B}} = \mathbf{V}^{\top}\mathbf{B}$  and  $\hat{\mathbf{B}}_d = \mathbf{V}^{\top}\mathbf{B}_d$
- Assemble past control inputs  $\mathbf{u}_k = \mathbf{u}(t_k; \mathbf{q}(t_k))$ :

$$\mathbf{U} = [\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_s]^\top \in \mathbb{R}^{s \times m},$$

**Reduced states**  $\hat{\mathbf{s}}_i := \mathbf{V}^{\top} \mathbf{s}(t_i)$  stored in

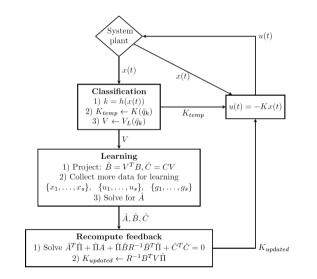
$$\hat{\mathbf{S}} = [\hat{\mathbf{s}}_1, \hat{\mathbf{s}}_2, \dots, \hat{\mathbf{s}}_\ell]^\top \in \mathbb{R}^{s \times r}$$

- $\blacksquare$  Derivative approximation  $\Rightarrow \dot{\hat{s}}_1, \ldots, \dot{\hat{s}}_\ell$
- $\blacksquare$  Operator inference problem for  $\hat{\mathbf{A}}=\hat{\mathbf{A}}(\tilde{\mathbf{q}})$ :

$$\min_{\hat{\mathbf{A}} \in \mathbb{R}^{r \times r}} \sum_{i=1}^{s} \left\| \dot{\hat{\mathbf{s}}}_{i} - \hat{\mathbf{A}} \hat{\mathbf{s}}_{i} - \hat{\mathbf{B}} \mathbf{u}_{i} \right\|_{2}^{2}$$

Convergence to projected matrices established [Peherstorfer and Willcox, 2016]

# Online: Detect subspace and learn model



Online classification gives
 "best-fit" low-dimensional
 subspace V<sub>L</sub>(q<sub>k</sub>) for learning

■ Learn/adapt new ROM system matrix Â(q) by incorporating real-time data

## Numerical example: Convection-diffusion PDE

Let 
$$\mathbf{x} = [x_1, x_2]^{\top} \in \Omega = [0, 1]^2$$
 and

$$\frac{\partial\theta}{\partial t}(t,\mathbf{x}) = q(t) \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right) \theta(t,\mathbf{x}) - x_2 \frac{\partial\theta}{\partial x_2}(t,\mathbf{x}) + b(\mathbf{x})u(t) + b_d g(t)$$

Boundary conditions:

$$\theta(t, x_1, 0) = 0, \quad \theta(t, 1, x_2) = 0, \quad \theta(t, x_1, 1) = 0, \quad \frac{\partial \theta}{\partial x_1}(t, 0, x_2) = 0$$

• Control enters through  $b(\mathbf{x}) = 5$  if  $x_1 \ge 1/2$  and 0 otherwise

• Uncertainty  $\Rightarrow$  diffusion coefficient  $q(t) \in \mathbb{R}$ 

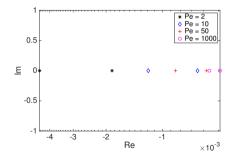
**Spatially discretized system** (piecewise linear FE):

$$\dot{\mathbf{s}}(t;q) = \mathbf{A}(q(t))\mathbf{s}(t;q) + \mathbf{B}\tilde{u}(t) + \mathbf{B}_d g(t), \quad \mathbf{s}(0) = \mathbf{s}_0 \in \mathbb{R}^n$$
$$y(t) = \mathbf{C}\mathbf{s}(t) \in \mathbb{R}$$

•  $\mathbf{C} = \frac{5}{n}[1, \dots, 1].$ • n = 3540 for FEM discretization = "truth model"

### Eigenvalues of A(Pe) for different Péclet numbers

- Parameter  $\bar{q}_i$  = Péclet number =  $\frac{\text{convective transport rate}}{\text{diffusive transport rate}}$
- High Péclet numbers indicate strongly convective flows
- Four Péclet numbers to generate library  $\mathcal{L}$ :  $Pe \in \{2, 10, 50, 1000\}$



**Figure:** The two eigenvalues with largest real part of the system matrix  $\mathbf{A}(\bar{q}_i)$ .

### Open loop output and gains for different Péclet numbers

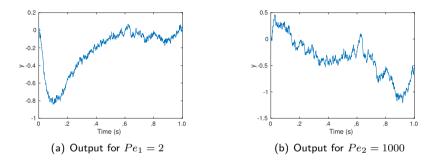
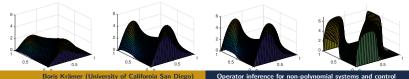


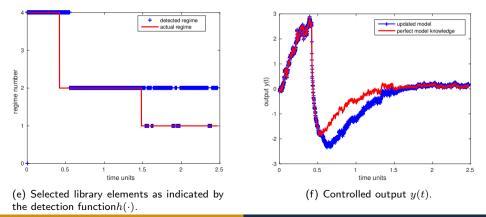
Figure: Output y(t) of the open loop convection diffusion system, excited with nonzero initial condition  $s_0(x, y) = 15 \sin(2\pi x) \sin(\pi y)$ ; disturbance  $g(t) \propto \mathcal{N}(0, 0.5)$  applied through a disturbance term at  $0 \le x_1 \le 0.05$ .



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#### Output with learned and intrusively-projected controller

- Simulate online until T = 2.5s
- Learning basis r = 10 (eigenbasis)
- Detection basis (POD) r = 30 from S = 1,000 snapshots
- $\blacksquare$  Misclassification after t>1.5s due to similar equilibrium solutions



### Numerical example II: Permeablity

Laplace equation on  $\Omega = [0,1]^2$  as model of flow through porous medium

$$\frac{\partial}{\partial t}\theta(t,\mathbf{x}) = \nu(t,\mathbf{x}) \cdot \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right)\theta(t,\mathbf{x}) + b(\mathbf{x})u(t) + b_d^1(\mathbf{x})g_1(t) + b_d^2(\mathbf{x})g_2(t)$$

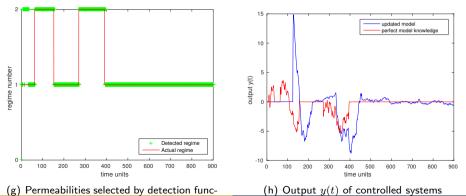
- $\blacksquare$  Uncertain permeability:  $q(t,\mathbf{x})=\nu(t,\mathbf{x})$
- **S**patial discretization:  $\mathbf{s} \in \mathbb{R}^n$ :

$$\dot{\mathbf{s}}(t) = \mathbf{A}(\mathbf{q}(t))\mathbf{s}(t) + \mathbf{B}u(t) + \mathbf{B}_d g(t)$$
$$y(t) = \mathbf{C}\mathbf{s}(t)$$

- White noise disturbance  $g(\cdot)$  enters through  $\mathbf{B}_d$  at  $[x_1, x_2] = [0.3, 0.3]$  and  $[x_1, x_2] = [0.3, 0.7]$
- Sensor location at  $[x_1, x_2] = [0.5, 0.6]$
- Control location at  $[x_1, x_2] = [0.6, 0.7]$
- $\blacksquare$  Compute library  ${\cal L}$  using three permeability fields  ${\bf q}_1({\bf x}), {\bf q}_2({\bf x}), {\bf q}_3({\bf x})$

#### Output of controlled system

- Learning basis  $V_L(\mathbf{q}_i)$ : Eigenbasis of order 20 for  $\mathbf{A}(\mathbf{q}_i), i = 1, 2, 3$
- Detection basis  $\mathbf{V}_D(\mathbf{q}_i)$ : POD basis of order 20 from closed-loop system excited with disturbances  $\mathbf{g}(t) = [g_1(t), g_2(t)]^{\top}$ . The system was simulated for 500s, and  $\ell = 10,000$  snapshots were used to compute the POD basis
- Stable regime 1, unstable regime 2



Operator inference for non-polynomial systems and control

## **Control performance**

- Case 1: Controller designed from projection-based ROM with perfect knowledge of q(t)
- Case 2: Controller designed from learned ROM (Operator Inference model)

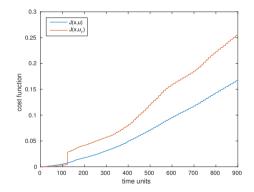
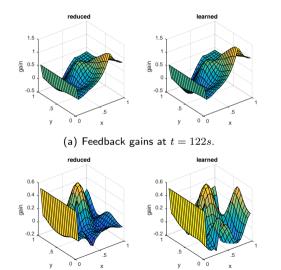


Figure: Control cost function  $J(\mathbf{s}, u)$  for both controllers on the full-order model.

#### Feedback gains: Intrusive ROM vs learned ROM



#### **Review:**

- **Situation:** A(q(t)) is not available online, neither are switching times  $t_i$
- Learning-based control framework for high-dimensional LPV system:
  - 1. Learning unknown ROM system matrix from data (Operator Inference)
  - 2. Detected switching time with localized subspace approach

#### **Conclusions:**

- Learning-based low-dimensional controller performs well and feedback gains are accurate
- Robustness to parametric changes can be addressed through online learning
- More robust controller designs could be obtained through  $(\mathcal{H}_{\infty})$

Feedback control for systems with uncertain parameters using online-adaptive reduced models. K./Peherstorfer/Willcox, SIAM J. on Applied Dynamical Systems 16(3), pp. 1563-1586, 2017.



# THANK YOU

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