From reduced-order modeling to scientific machine learning

How computational science is enabling the design of next-generation aerospace systems

Professor Karen E. Willcox
SDM Lecture | January 5, 2022

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FOR COMPUTATIONAL ENGINEERING & SCIENCES

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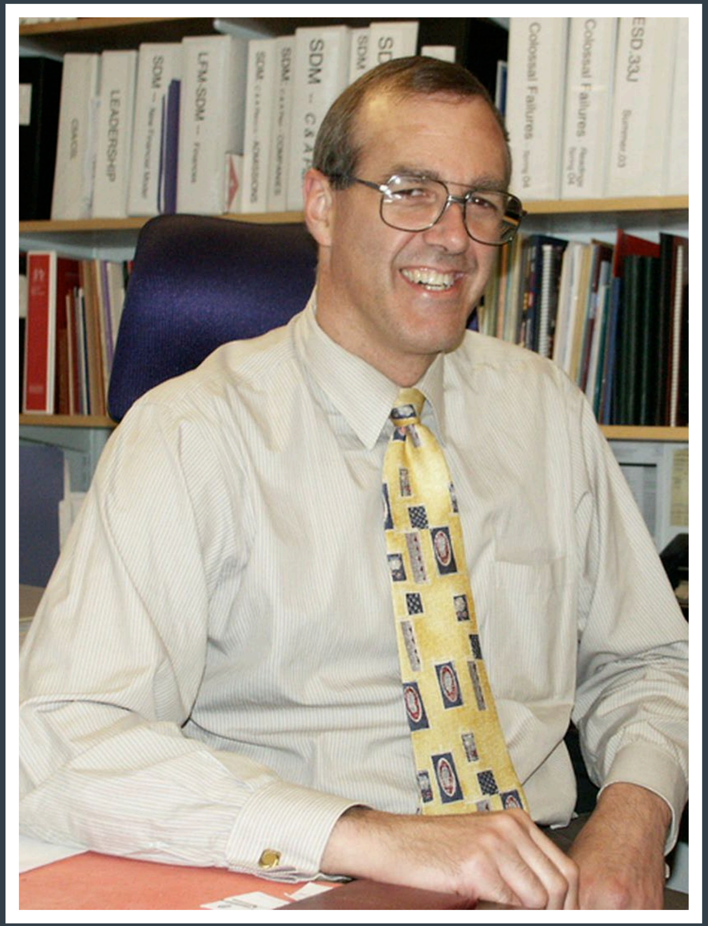

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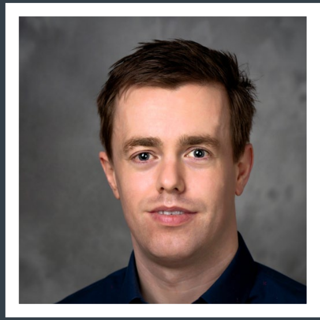

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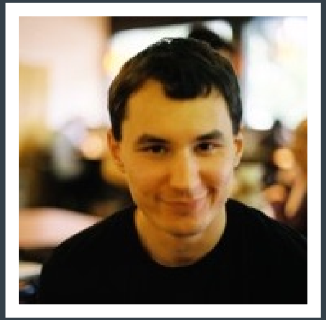

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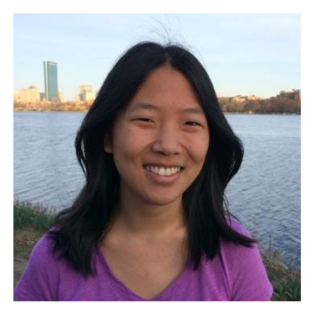

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Outline

1 **Learning from data**

The imperative of physics-based modeling & inverse theory

2 **Reduced-order modeling**

A critical enabler for accelerating predictive computations in support of engineering design

3 **Operator Inference**

Combining model reduction & machine learning to learn predictive reduced-order models

4 **Outlook**

Forward simulations
The backbone of engineering analysis

Uncertainty quantification
Design for reliability & robustness

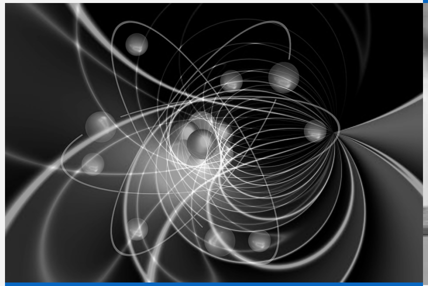
Optimization
Optimal design, inverse problems, control, parameter estimation

Scientific machine learning
Blending physics modeling & data-driven learning

Computational science has been enabling engineering design for six decades

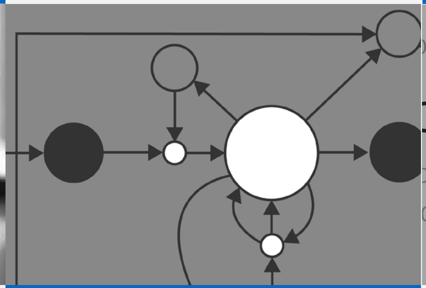
Scientific Machine Learning

What are the opportunities and challenges of machine learning in complex applications across science, engineering, and medicine?



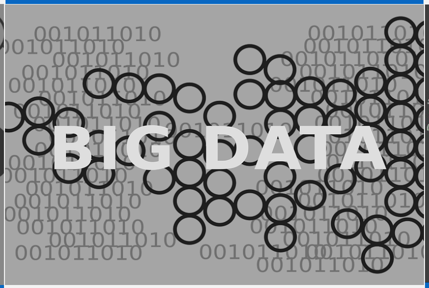
Respect physical constraints

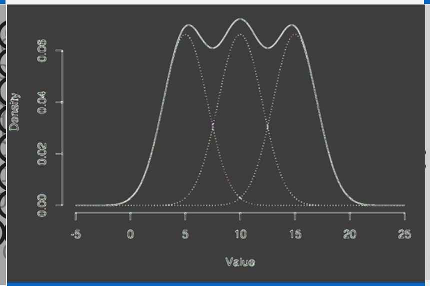
Embed domain knowledge



Bring interpretability to results

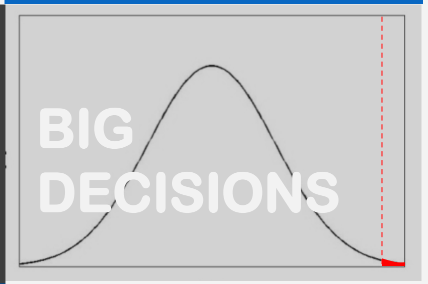
Integrate sparse, heterogeneous, noisy & incomplete data





Make predictions with quantified uncertainties

Support high-consequence decisions



https://xkcd.com/1838/

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Check for updates

The imperative of physics-based modeling and inverse theory in computational science

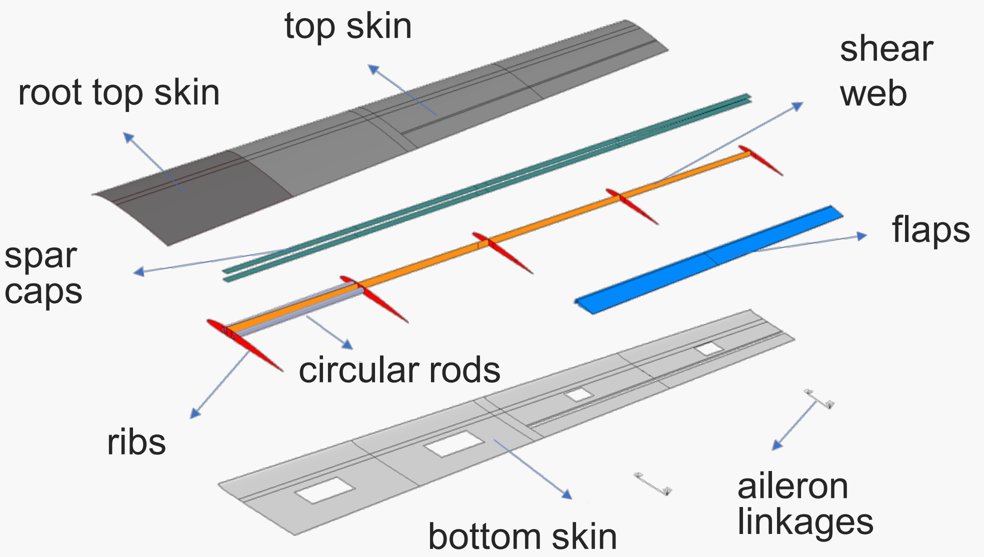
To best learn from data about large-scale complex systems, physics-based models representing the laws of nature must be integrated into the learning process. Inverse theory provides a crucial perspective for addressing the challenges of ill-posedness, uncertainty, nonlinearity and under-sampling.

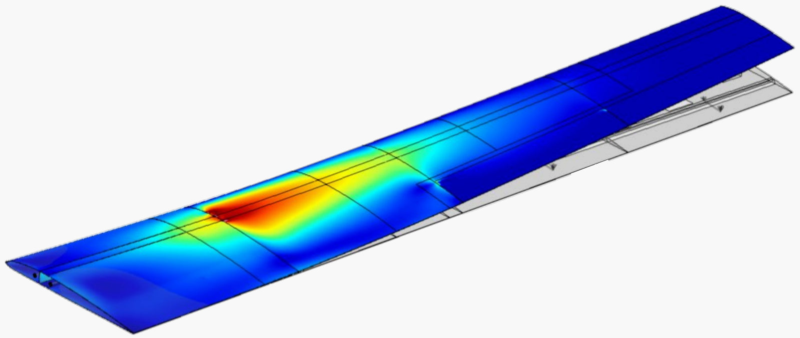
Karen E. Willcox, Omar Ghattas and Patrick Heimbach

The notions of 'artificial intelligence (AI) for science' and 'scientific machine learning' (SciML) are gaining widespread attention in the scientific community. These initiatives target development and adoption of AI approaches in scientific and engineering fields with the goal of accelerating research and development breakthroughs in energy, basic science, engineering, medicine and national security. For the past six decades, these fields have been advanced through the synergistic and principled use of geological processes evolve. Physics-based models typically encode knowledge in the form of conservation and constitutive laws, often based on decades if not centuries of theoretical development and experimental validation. These laws often manifest as systems of differential equations that are solved numerically with high-performance computing (HPC).

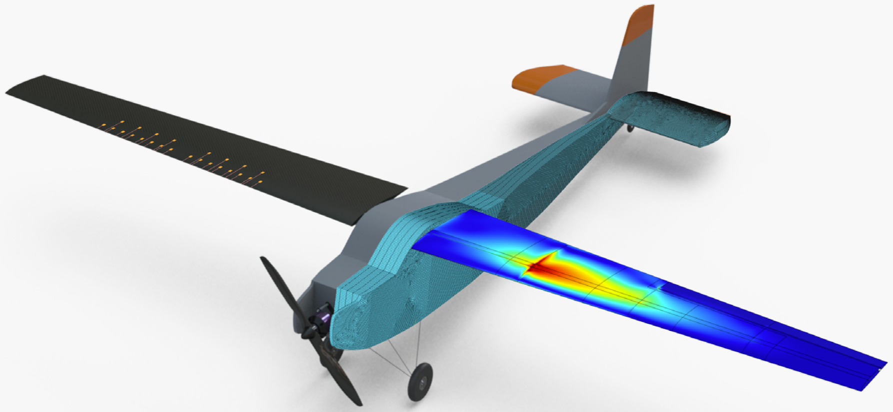
In his famous 1960 article, Eugene Wigner wrote about 'The unreasonable effectiveness of mathematics in the natural sciences'[2], pointing to "the 'laws of nature' constraints, purely data-driven approaches are unlikely to be predictive, no matter how expressive the underlying representation. Even when physical models are not well-established (such as for many biological processes, in constitutive laws for complex materials, or in subgrid scale models for unresolved physics), we know that certain universal properties and relationships must hold, such as conservation properties, material frame indifference, objectivity, symmetries, or other invariants. The learning-from-data

PHYSICS-BASED MODELS are POWERFUL and bring PREDICTIVE CAPABILITIES





but they can be COMPUTATIONALLY EXPENSIVE



COMPUTATIONAL SCIENCE enables **AEROSPACE DESIGN**

1 **Learning from data**

The imperative of physics-based modeling & inverse theory

2 **Reduced-order modeling**

A critical enabler for accelerating predictive computations in support of engineering design

3 **Operator Inference**

Combining model reduction & machine learning to learn predictive reduced-order models

4 **Outlook**

Reduced-order models are critical enablers for data-driven learning & engineering design

high-fidelity physics-based simulation

projection-based reduced-order model

dimension $10^3 - 10^9$
solution time ~minutes / hours / days

dimension $10^1 - 10^3$
solution time ~seconds / minutes

1 **Train**: Solve PDEs to generate training data (snapshots)

2 **Identify structure**: Compute a low-dimensional basis

3 **Reduce**: Project PDE model onto the low-dimensional subspace

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Technical Notes

TECHNICAL NOTES are short manuscripts describing new developments or important results of a preliminary nature. These Notes cannot exceed 6 manuscript pages and 3 figures; a page of text may be substituted for a figure and vice versa. After informal review by the editors, they may be published within a few months of the date of receipt. Style requirements are the same as for regular contributions (see inside back cover).

An Approximate Analysis Technique for Design Calculations

R. L. Fox* and H. Miura†
Case Western Reserve University, Cleveland, Ohio

1 Introduction

In the design of complex structures, it is often necessary or desirable to employ approximations in the analysis to reduce computational cost and required computer storage. In automated or computer assisted design applications, it is often necessary to analyze a considerable number of designs, and it is the computational cost of these analyses that inhibits applications in many cases. Although no specific optimization problem is formulated in this Note, the method proposed is particularly applicable to such problems.

In this Note, a simple method is proposed with which one can obtain approximate results for analyses of modified designs based upon a limited number of exact analysis results. The idea of this method is based on the practically experienced fact that the number of design variables are usually far smaller than the degrees of freedom of the system, and the further observation that often large numbers of analysis degrees of freedom are dictated by the topology of the design rather than by the expected complexity of its behavior.

Some encouraging numerical examples, computed for space truss structures, are presented.

2 Approximate Method

In the static analysis of a structure using the displacement method, the system is expressed in the form

$$\underset{n\times n}{K}\ \underset{n\times 1}{X} = \underset{n\times 1}{P} \qquad (1)$$

where K is the stiffness matrix, X is the vector of displacement degrees of freedom, and P is the load vector. If the structure has t design variables $(d_1, d_2, \ldots d_t)$, we can consider this set as a vector D in t-dimensional space. In this design space, consider the r "basic" designs given by a set of the design vectors $D_1, D_2, \ldots D_r$. Corresponding to these basic design vectors, the stiffness matrices $K_1, K_2, \ldots K_r$ are obtained, and by solving the r sets of simultaneous equations,

$$K_i X_i = P, \ i = 1, 2, \ldots, r \qquad (2)$$

basic displacement vectors $X_1, X_2, \ldots X_r$ are computed.

Table 1 Basic designs

Member	Design 1	Design 2	Design 3	Design 4	Design 5
1 ~ 18	1.0in.²	0.2in.²	1.0in.²	1.0in.²	1.0in.²
19 ~ 42	1.0	1.0	0.3	1.0	1.0
43 ~ 72	2.0	2.0	2.0	0.4	2.0
73 ~ 124	0.5	0.5	0.5	0.5	0.1

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† Graduate Assistant.

Consider now a new design vector D_N in the nei… of the basic design vectors. The stiffness matrix c… ing to D_N can be computed as K_N, and the exact dis… vector due to the external load P would ordinar… tained by solving a set of simultaneous equations:

$$K_N X_N = P$$

Here it is assumed that X_N can be approxima… linear combination of basic displacement vectors … X_r.

$$X_N \simeq \tilde{X}_N = y_1X_1 + y_2X_2 + \ldots + y_rX_r$$

If $X_1, X_2, \ldots X_r$ are linearly independent and $r = n$ … the exact solution, but we are now considering a c… n. In matrix form, Eq. (4) will be expressed

$$\tilde{X}_N = TY$$

where

$$\underset{n\times r}{T} = [X_1, X_2, \ldots X_r]$$

$$\underset{r\times 1}{Y} = \begin{Bmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ \cdot \\ y_r \end{Bmatrix}$$

The vector Y is then determined by solving a s… of Eqs. (6), which is obtained by substituting E… Eq. (3) assuming $\tilde{X}_N \cong X_N$ and premultiplying … T^T, i.e.,

$$\underset{r\times n}{T^T}\ \underset{n\times n}{K_N}\ \underset{n\times r}{T}\ \underset{r\times 1}{Y} = \underset{r\times n}{T^T}\ \underset{n\times 1}{P}$$

Introducing the notation

$$K_R = T^T K_N T; \quad P_R = T^T P$$

we have

$$\underset{r\times r}{K_R}\ \underset{r\times 1}{Y} = \underset{r\times 1}{P_R}$$

In short, an approximate displacement vector $\tilde{X}_N$ …

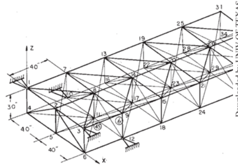

Fig. 1 Example structure.

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Reduced Basis Technique for Nonlinear Analysis of Structures

80004

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A reduced basis technique and a computational algorithm are presented for predicting the nonlinear static response of structures. A total Lagrangian formulation is used and the structure is discretized by using displacement finite element models. The nodal displacement vector is expressed as a linear combination of a small number of basis vectors and a Rayleigh-Ritz technique is used to approximate the finite element equations by a reduced system of nonlinear equations. The Rayleigh-Ritz approximation functions (basis vectors) are chosen to be those commonly used in the static perturbation technique namely, a nonlinear solution and a number of its path derivatives. A procedure is outlined for automatically selecting the load (or displacement) step size and monitoring the solution accuracy. The high accuracy and effectiveness of the proposed approach is demonstrated by means of numerical examples.

Nomenclature

A	= cross sectional area
E	= Young's modulus of the material
e	= error norm defined by Eq. (16)
$\{f(X,q)\}$ and $\{\tilde{f}(\psi,q)\}$	= vectors defined in Eqs. (1) and (4), respectively
G	= shear modulus of the material
$\{G(X)\}$	= vector of nonlinear terms
$\{\tilde{G}(\psi)\}$	= vector of nonlinear terms of the reduced system
h	= arch thickness
I	= moment of inertia
$[K]$	= linear global stiffness matrix of the structure
$[\tilde{K}]$	= linear stiffness matrix of the reduced system
$\tilde{K}_{ij}$	= $\tilde{K}_{ij} + \partial G_i/\partial X_j$
L	= length of beam
ℓ_1, ℓ_2	= lengths of vectors $\{X\}$ and $\{\dot{X}\}$
$[\mathfrak{M}]$	= Gram matrix of basis vectors
N	= normal force
n	= total number of degrees-of-freedom in the finite element model
P	= applied concentrated load
$\{Q\}$	= normalized external load vector
$\{\tilde{Q}\}$	= normalized load vector of the reduced system
q	= load parameter
R	= local radius of curvature of the arch
$\{R\}$	= residual vector defined by Eq. (15)
r	= number of basis vectors (reduced degrees-of-freedom)
$S_{(i)}$	= current stiffness parameter corresponding to ith load (or displacement) increment
U	= total strain energy
u, w	= tangential (circumferential) a… (radial) displacement compo… center line of the arch
$\{X\}$	= vector of unknown nodal disp…
$\{\bar{X}\}_i \ (i=1 \text{ to } r)$	= basis vectors
$\{\dot{X}\}, \{\ddot{X}\}, \{\dddot{X}\}$	= derivatives of $\{X\}$ with res… parameter λ
β	= condition number of $[\mathfrak{M}]$
$[\Gamma]$	= matrix of basis vectors
θ	= half subtended angle of the ar…
λ	= path parameter
$\{\psi\}$	= vector of undetermined coeffi…

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Index categories: Structural Design; Structural Stability; Structural Statics.
*Professor of Engineering and Applied Science. Associate Fellow AIAA.
†Programmer Analyst.

Introduction

Large deflection nonlinear analysis has rec… the focus of intense efforts because of the i… of new lightweight materials (such as fibrous co… aircraft and aerospace structures and the harsh … to which these structures are often subjected. … progress has been made in the development of … powerful finite element discretization methods … improved numerical methods and programmin… for nonlinear analysis of structures (see, for exam… 4). In spite of these advances, the solutions of mo… nonlinear structural problems require excessive … computer time and, therefore, are not economica…

The large numbers of degrees-of-freedom … structural systems are often dictated by their top… than by the expected complexity of the behavior. … been recognized and used to advantage in au… timum design and vibration analysis[5-7] and mo… nonlinear analysis.[8-11] In the latter case a hybrid … been used which combines contemporary finite … classical Rayleigh-Ritz approximations, thereb… the modeling versatility inherent in the finite ele… and, at the same time, reducing the number o… freedom through Rayleigh-Ritz approximation.

Since the effectiveness of this approach f… analysis depends, to a great extent, on the appro… of the Rayleigh-Ritz approximation functions … tors, it will be referred to herein as reduced basis … Refs. 8-10, the linear bifurcation buckling modes … basis vectors and only mildly nonlinear pr… considered. In contrast, Ref. 11 used the linear … corrections to it as basis vectors and presented a… controlling the errors in nonlinear analysis.

The aforementioned choices for basis vectors c… to realize the full potential of the reduced basis t… the one hand, the generation of bifurcation …

Annu. Rev. Fluid Mech. 2001. 33:445–90

Modeling of Fluid-Structure Interaction

Earl H Dowell and Kenneth C Hall
Department of Mechanical Engineering and Materials Science, Edmund T. Pratt, Jr. School of Engineering, Duke University, Durham, North Carolina 27708-0300; e-mail: dowell@mail.ee.duke.edu, KennethC.Hall@euler.egr.duke.edu

Key Words time linearization, nonlinear dynamics, reduced-order models, aeroelasticity

■ **Abstract** The interaction of a flexible structure with a flowing fluid in which it is submersed or by which it is surrounded gives rise to a rich variety of physical phenomena with applications in many fields of engineering, for example, the stability and response of aircraft wings, the flow of blood through arteries, the response of bridges and tall buildings to winds, the vibration of turbine and compressor blades, and the oscillation of heat exchangers. To understand these phenomena we need to model both the structure and the fluid. However, in keeping with the overall theme of this volume, the emphasis here is on the fluid models. Also, the applications are largely drawn from aerospace engineering although the methods and fundamental physical phenomena have much wider applications. In the present article, we emphasize recent developments and future challenges. To provide a context for these, the article begins with a description of the various physical models for a fluid undergoing time-dependent motion, then moves to a discussion of the distinction between linear and nonlinear models, time-linearized models and their solution in either the time or frequency domains, and various methods for treating nonlinear models, including time marching, harmonic balance, and systems identification. We conclude with an extended treatment of the modal character of time-dependent flows and the construction of reduced-order models based on an expansion in terms of fluid modes. The emphasis is on the enhanced physical understanding and dramatic reductions in computational cost made possible by reduced-order models, time linearization, and methodologies drawn from dynamical system theory.

CONTENTS

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Our Operator Inference approach blends model reduction & machine learning

- A **physics-based model**
  Typically described by PDEs or ODEs
- Lens of **projection** to define the form of a structure-preserving low-dimensional model

Define the **structure of the reduced model**

$$\dot{\hat{\mathbf{x}}} = \widehat{\mathbf{A}}\hat{\mathbf{x}} + \widehat{\mathbf{B}}\mathbf{u} + \widehat{\mathbf{H}}(\hat{\mathbf{x}} \otimes \hat{\mathbf{x}})$$

↓

Non-intrusive learning by inferring reduced model operators $\widehat{\mathbf{A}}, \widehat{\mathbf{B}}, \widehat{\mathbf{H}}$ from simulation data

Learning from data through the lens of a reduced-order physics-based model

[Peherstorfer & Willcox, CMAME 2016]

What is a physics-based model?

A representation of the **governing laws of nature** that innately embeds the concepts of **time, space, and causality**

In solving the governing equations of the system, we constrain the **predictions** to lie on the **solution manifold** defined by the laws of nature

Example: equations of linear elasticity

$$\rho \frac{\partial^2 u}{\partial t^2} = \frac{\partial \sigma}{\partial x} + \frac{\partial \sigma}{\partial y} + F$$

equation of motion (Newton's 2nd law)

$$\varepsilon = \frac{1}{2}[\nabla u + (\nabla u)^{\mathsf{T}}]$$

strain-displacement equations

$$\sigma = C : \varepsilon$$

constitutive equations

\+ boundary conditions
\+ initial conditions

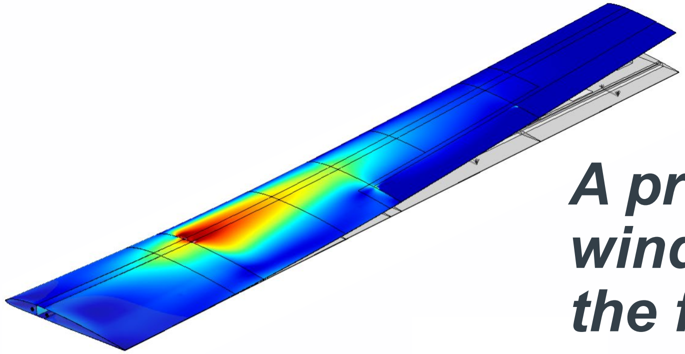
a mathematical model of how solid objects deform, relating stress σ, strain ε, displacement u, and loading F

The unreasonable effectiveness of physics-based models [Wigner, 1960]

Solving a physics-based model:

Given initial conditions, boundary conditions, loading conditions, and system parameters

Compute solution trajectories $\sigma(x, y, t), \varepsilon(x, y, t), \mathrm{u}(x, y, t), \ldots$



A predictive window on the future

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strain-displacement equations

$$\sigma = C : \varepsilon$$

constitutive equations

+ boundary conditions
+ initial conditions

a mathematical model of how solid objects deform, relating stress σ, strain ε, displacement u, and loading F

A mathematical model solved with computational science

Discretize: Spatially discretized computational fluid dynamic (CFD) model

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

discretized **state x** contains physical states at N_z spatial grid points – $N_z \sim O(10^4 - 10^6)$

$$\mathbf{x} = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ \vdots \\ u_{N_z} \end{bmatrix}$$

e.g., nodal displacements

Projecting a linear system

Full-order model (FOM)
state $\mathbf{x} \in \mathbb{R}^N$

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u}$$

Approximate
$\mathbf{x} \approx \mathbf{V}\mathbf{x}_r$
$V \in \mathbb{R}^{N \times r}$

Residual: N eqs $\gg r$ dof

$$\mathbf{r} = \mathbf{V}\dot{\mathbf{x}}_r - \mathbf{A}\mathbf{V}\mathbf{x}_r - \mathbf{B}\mathbf{u}$$

Project
$\mathbf{W}^\top \mathbf{r} = 0$
(Galerkin: $\mathbf{W} = \mathbf{V}$)

Reduced-order model (ROM)
state $\mathbf{x}_r \in \mathbb{R}^r$

$$\dot{\mathbf{x}}_r = \mathbf{A}_r\mathbf{x}_r + \mathbf{B}_r\mathbf{u}$$

$$\mathbf{A}_r = \mathbf{V}^\top \mathbf{A}\mathbf{V}$$
$$\mathbf{B}_r = \mathbf{V}^\top \mathbf{B}$$

Linear Model

FOM: $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u}$

$\downarrow$

ROM: $\dot{\mathbf{x}}_r = \mathbf{A}_r\mathbf{x}_r + \mathbf{B}_r\mathbf{u}$

Precompute the ROM matrices:

$$\mathbf{A}_r = \mathbf{V}^\top\mathbf{A}\mathbf{V},\ \ \mathbf{B}_r = \mathbf{V}^\top\mathbf{B}$$

Quadratic Model

FOM: $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{H}(\mathbf{x} \otimes \mathbf{x}) + \mathbf{B}\mathbf{u}$

$\downarrow$

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

Precompute the ROM matrices and tensor:

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

projection preserves structure $\longleftrightarrow$ structure embeds physical constraints

COMPUTATIONAL SCIENCE enables AEROSPACE DESIGN

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4 **Outlook**

The Operator Inference problem

Given (1) a physical/natural system with known governing equations, and (2) a set of data in the form of state snapshots (experimental or simulation)

Infer a reduced-order model that recovers the given data and provides a predictive capability to rapidly simulate unseen conditions

$$\min_{\mathbf{O}} ||\mathbf{DO} - \mathbf{R}||$$

$\mathbf{O}$: low-dimensional operators that define the reduced model

$\mathbf{D}, \mathbf{R}$: data matrix / forcing from simulation and/or experimental data

We will use:

- the **physics** to define the structured form of the model we seek
- **projection-based model reduction** to cast the inference in a reduced coordinate space and to provide error estimates in some settings
- **inverse theory** to analyze the structure of the resulting problem and treat it numerically
- **numerical linear algebra** to achieve efficient scalable algorithms

Our Operator Inference approach blends model reduction & machine learning

1. A **physics-based model**
   Typically described by PDEs or ODEs
2. Lens of **projection** to define the form of a structure-preserving low-dimensional model

Define the **structure of the reduced model**

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

Non-intrusive learning by inferring reduced operators from simulation data [Peherstorfer & W., 2016]

snapshots generated from projected simulation data

low-dimensional operators define the reduced model as a dynamical system

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

minimum residual formulation leads to linear least squares

- Regularization is key [McQuarrie, Huang & W., 2021]
- If data are Markovian, Operator Inference **recovers the intrusive POD ROM** [Peherstorfer, 2020]

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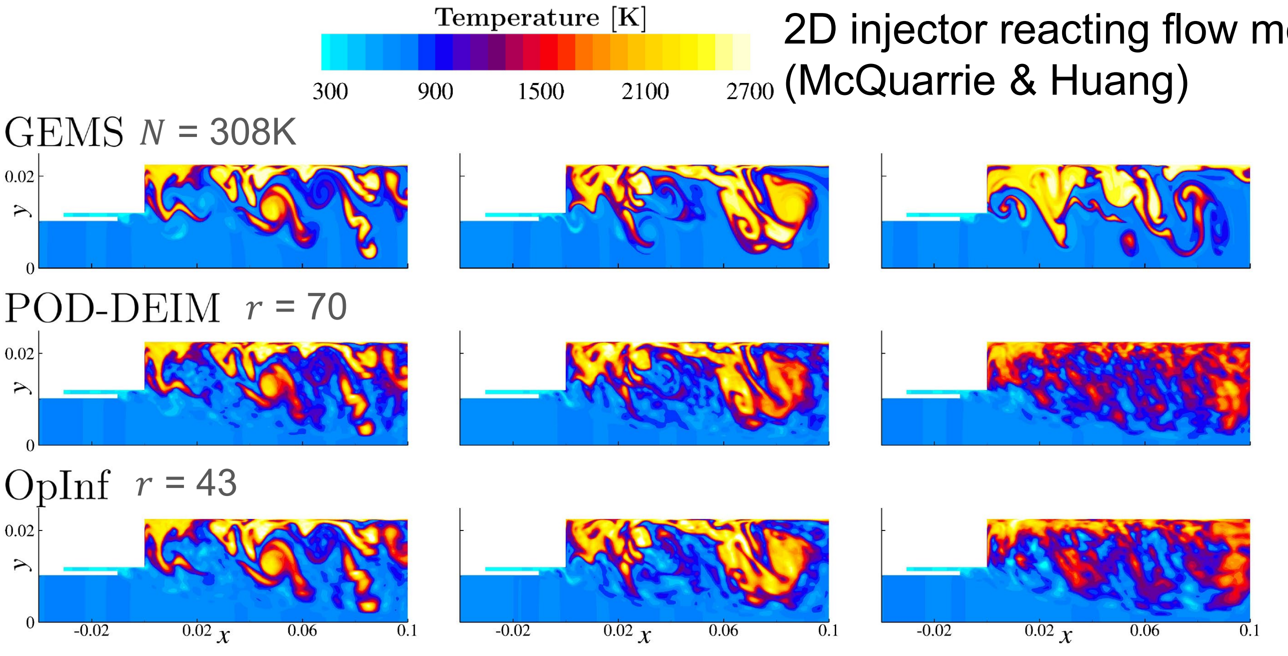
Non-intrusive learning by inferring reduced operators from simulation data [Peherstorfer & W., 2016]

Operator Inference is non-intrusive; requires only snapshot data

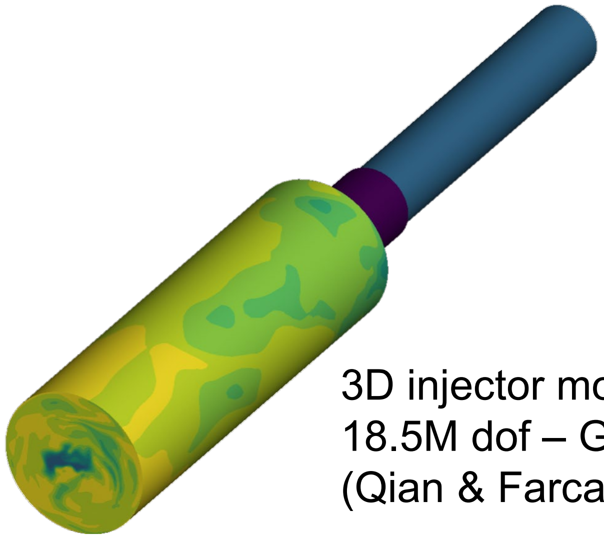
1. Generate snapshots from high-fidelity simulation
2. Compute POD basis (SVD) and snapshot low-dimensional representation
3. Solve linear least squares minimization problem to infer the low-dimensional model

Operator Inference ROMs are competitive in accuracy with state-of-the-art intrusive ROMs but are much faster/simpler to implement and faster to solve

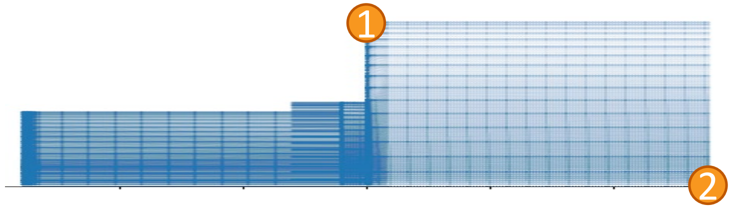


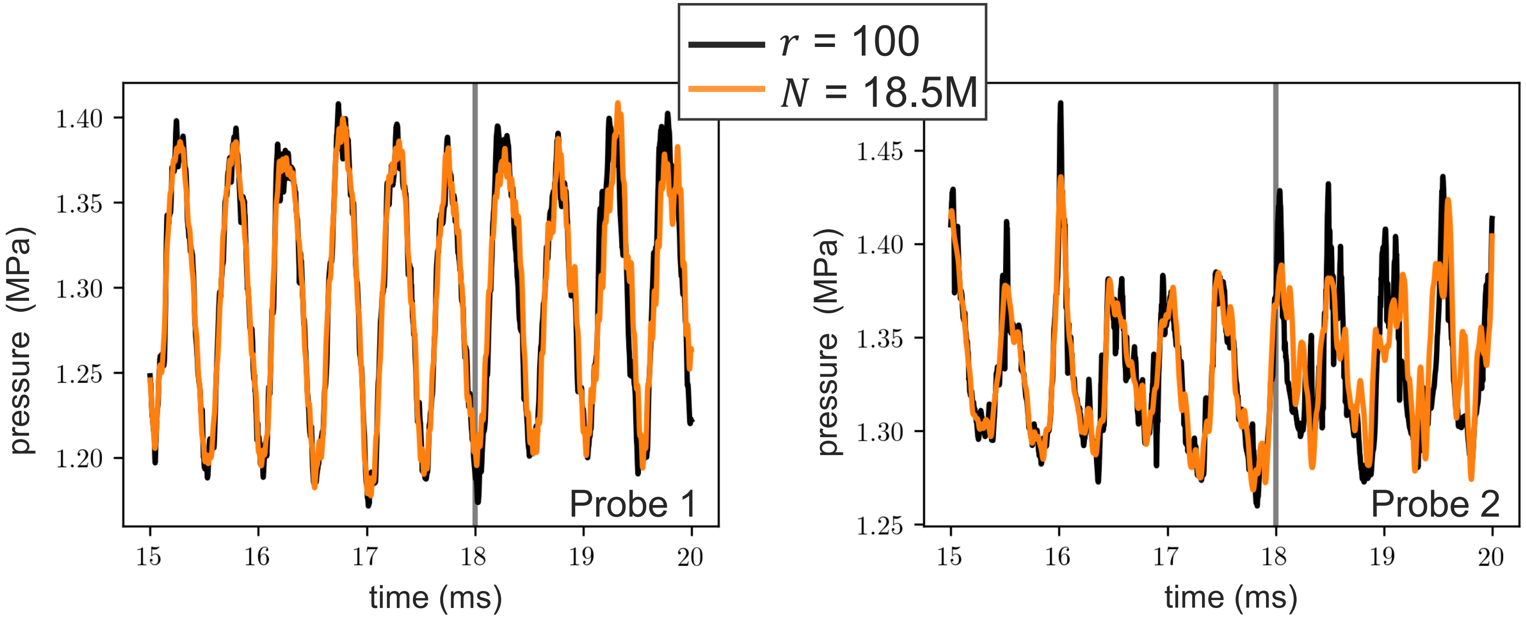
(a) $t = t_{15,000} = 0.0165$ s. (b) $t = t_{20,000} = 0.0170$ s. (c) $t = t_{25,000} = 0.0175$ s.

2D injector reacting flow model (McQuarrie & Huang)

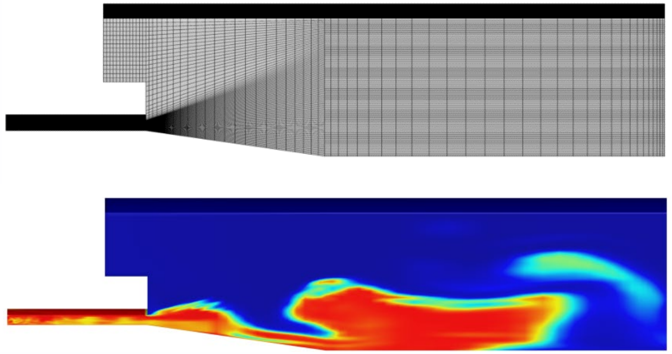


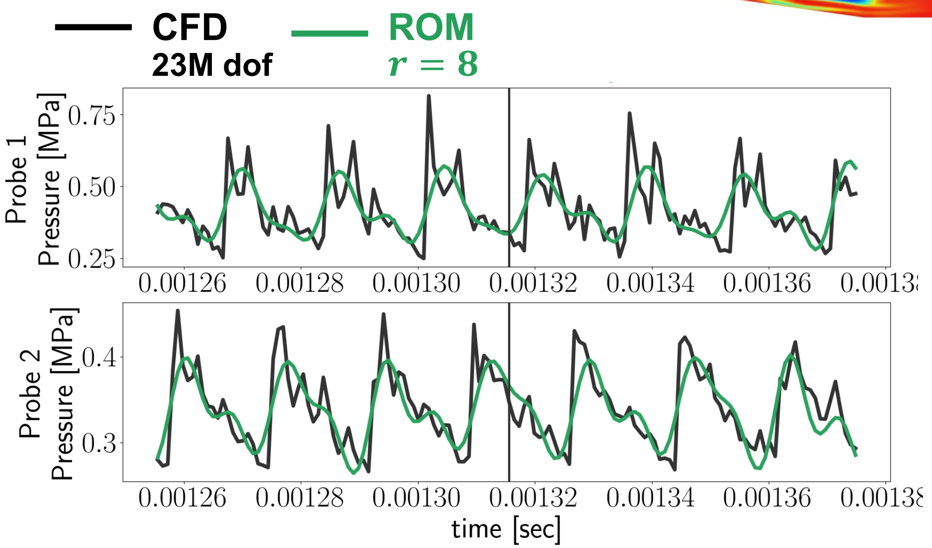
3D injector model
18.5M dof – GEMS
(Qian & Farcas)

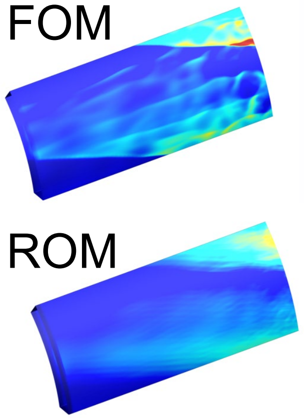




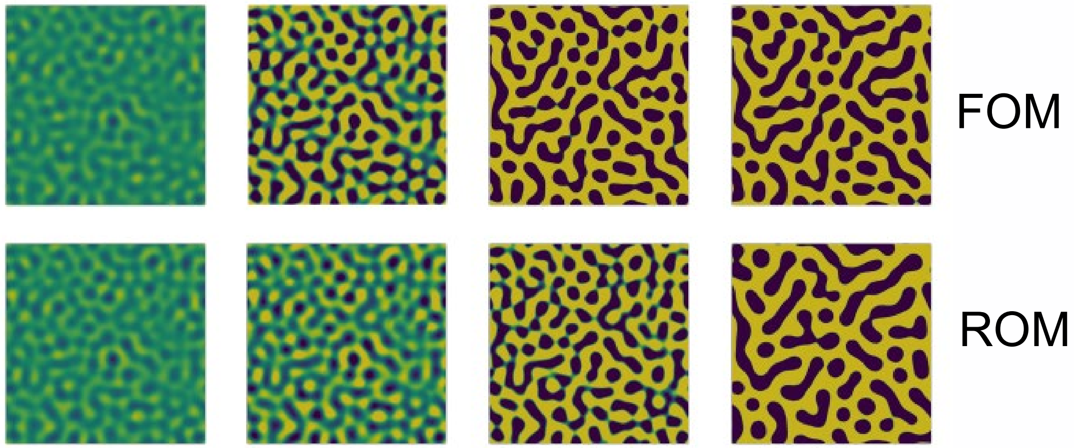
Rotating Detonation Engine (Farcas)



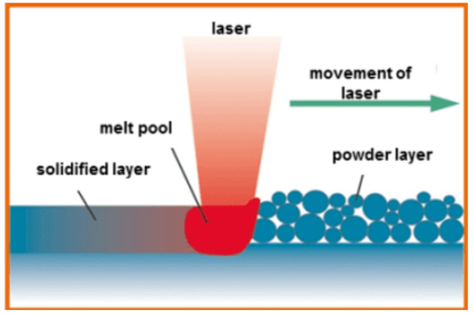




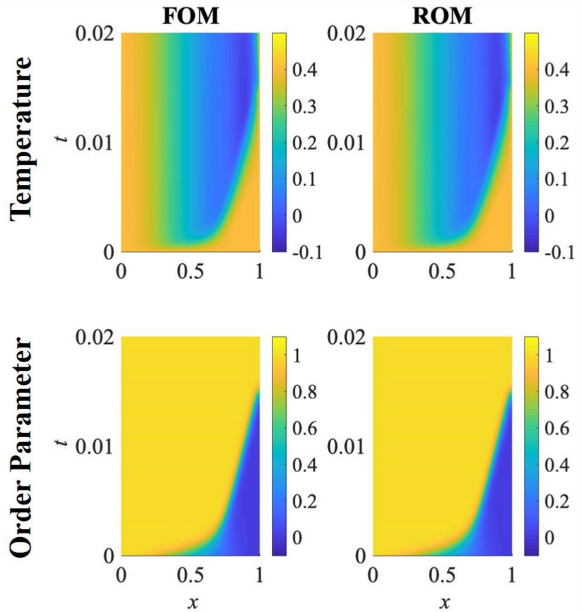
Phase-field modeling (Geelen)



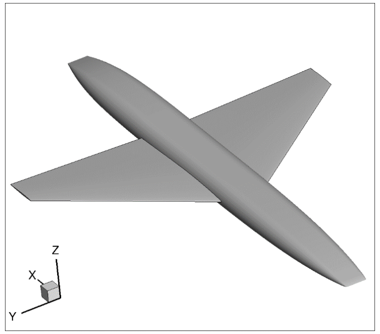
Solidification in additive manufacturing (Khodabakhshi)

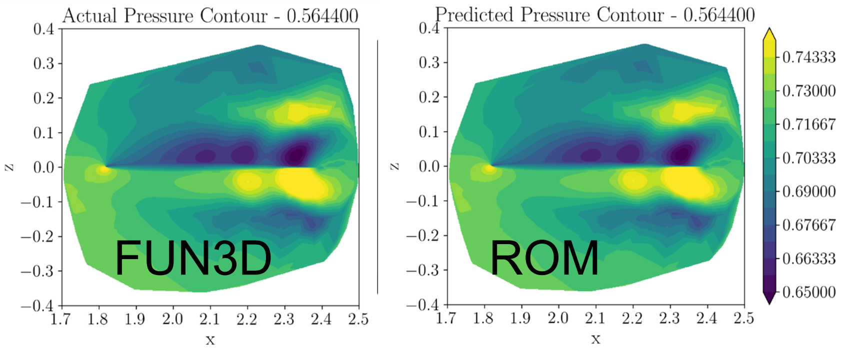


https://www.bintoa.com/powder-bed-fusion



VAT Wing (Zastrow & Chaudhuri)





Structure + predictivity
from physics

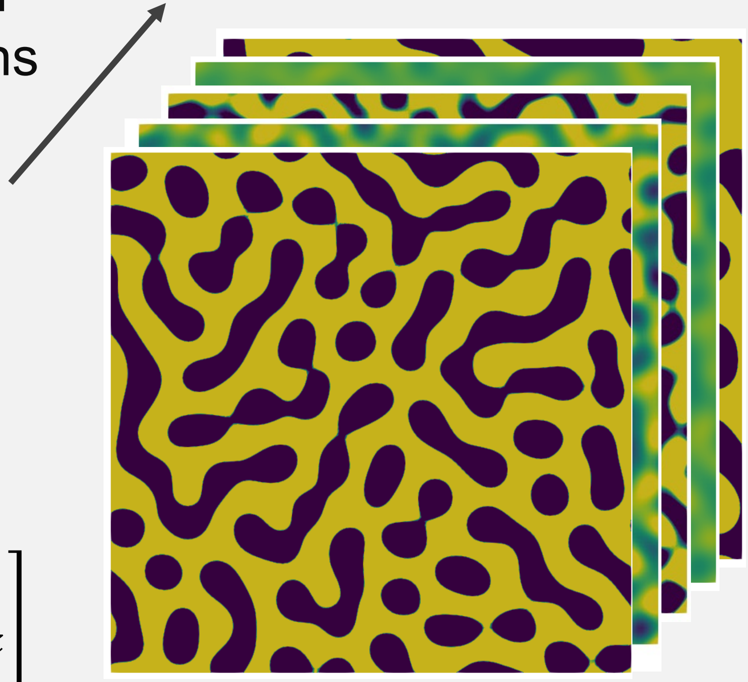
Non-intrusivity + flexibility
from machine learning

Operator Inference

What more can machine learning concepts bring to model reduction?

Why are many aerospace problems challenging for model reduction?

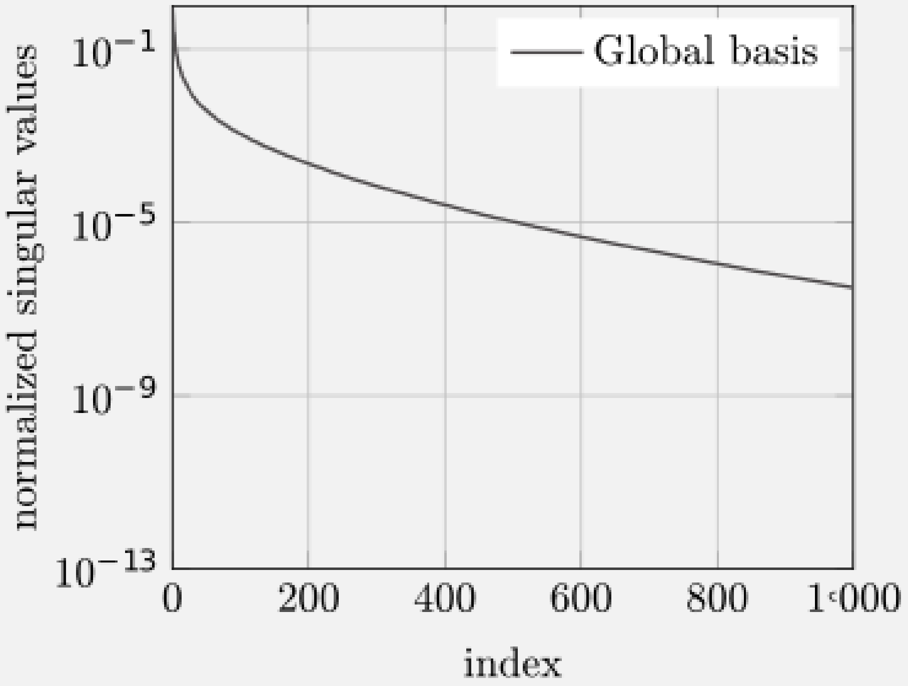
Snapshot collection across different time steps and initial conditions



$$\mathbf{S} = \begin{bmatrix} | & | & & | \\ \mathbf{s}_0 & \mathbf{s}_1 & \cdots & \mathbf{s}_k \\ | & | & & | \end{bmatrix}$$

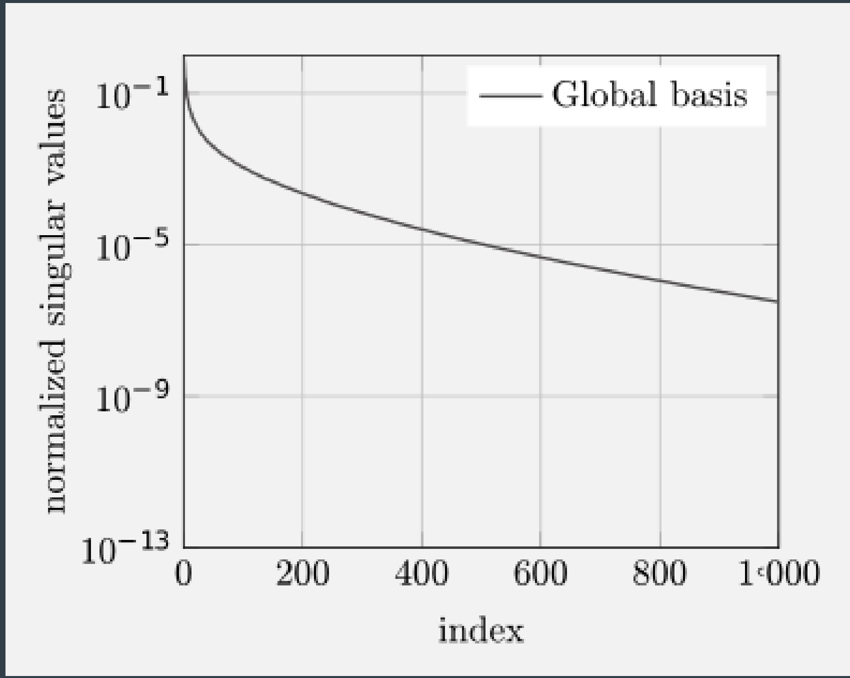
Cahn-Hilliard phase-field model

Slow decay of the singular values
→ reduced model has high dimension



Constructing reduced-order models is challenging for advection-dominated and multiscale problems

- Addressed by: adaptive model reduction, interpolation, nonlinear manifolds, dictionaries of ROMs, problem-specific registration, domain decomposition, …
  [Amsallem, Beran, Farhat, Haasdonk, Ohlberger, Patera, Peherstorfer, Rozza, Ryckelynck, Stamm, Vega, Zahr, …]
- These approaches are all intrusive, limiting their applicability



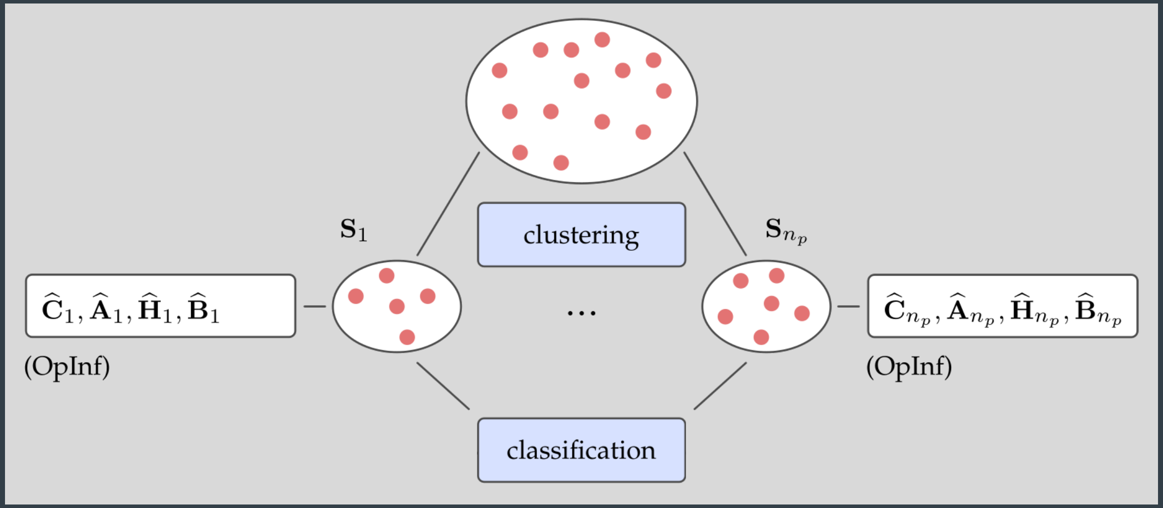
→ **Localized Operator Inference:**
non-intrusive physics-based (Operator Inference) **+**
approximation power of **dictionaries of localized ROMs**

Localized Operator Inference – Divide & Conquer

[Geelen & W., Phil. Trans. Royal Society A, 2021]

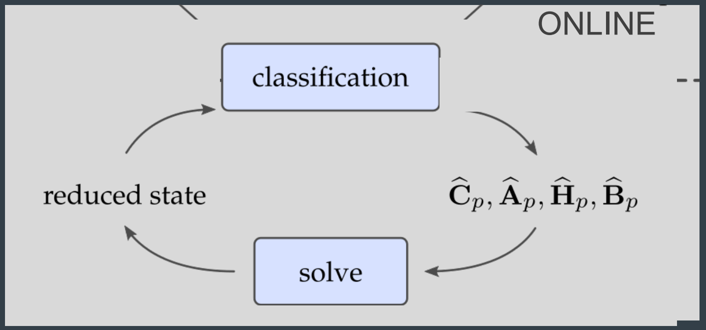
Offline

1. **Data collection & clustering**
   using unsupervised learning methods
2. **Train a classifier**
   for selecting the local ROM
3. **Learn a set of cluster-specific ROMs**



Online

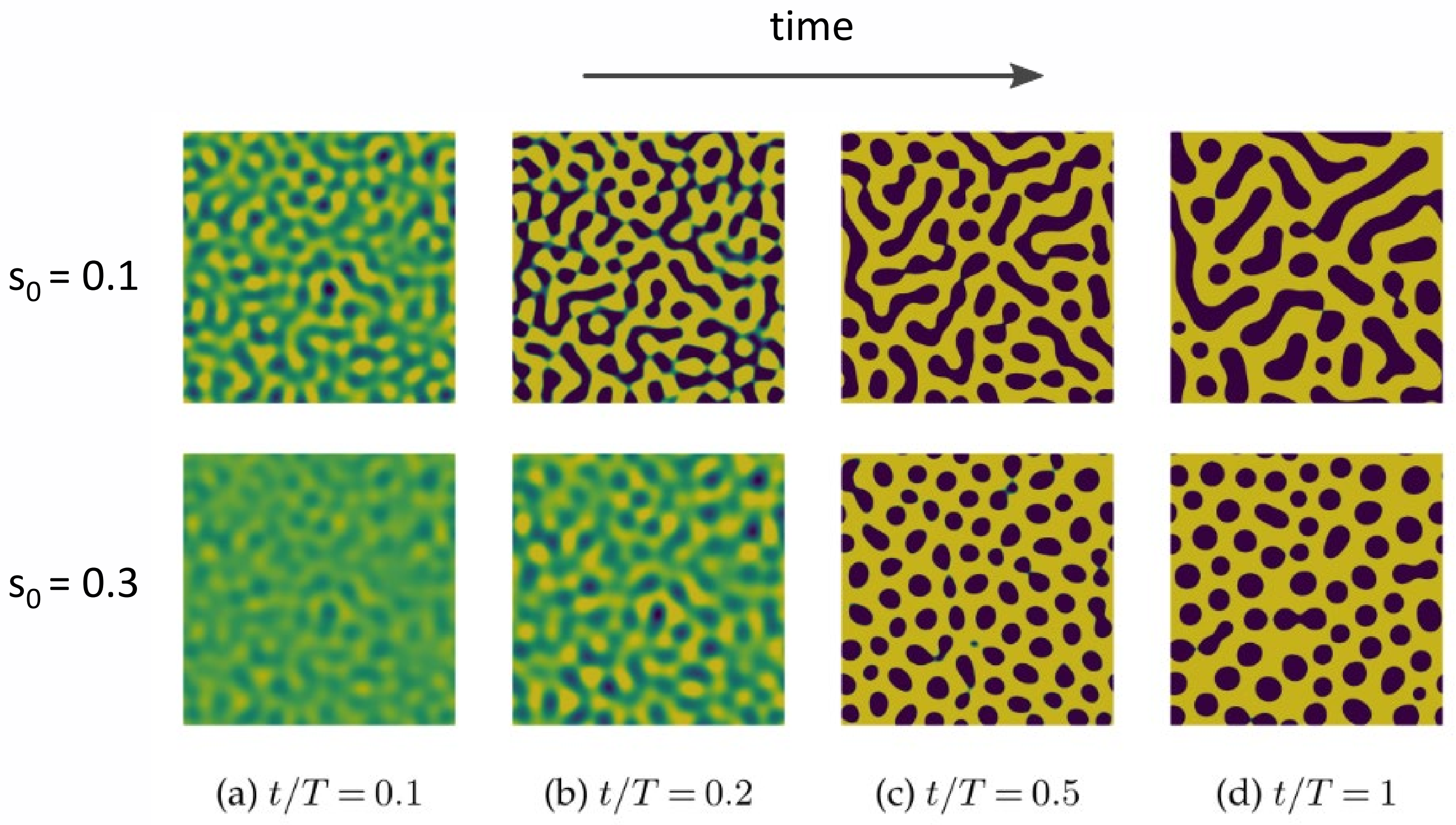
1. **Select ROM** – using the state as an indicator, select which local ROM to employ
2. **Solve** – evaluate the ROM using reduced model operators corresponding to the selected local ROM



Reducing a Cahn-Hilliard phase-field model

$$\frac{\partial}{\partial t}s(\mathbf{x},t) = M\nabla^2\left(s^3(\mathbf{x},t) - s(\mathbf{x},t) - \ell\nabla^2 s(\mathbf{x},t)\right)$$

Different initial conditions give rise to different kinematics across different **temporal** and **spatial** scales



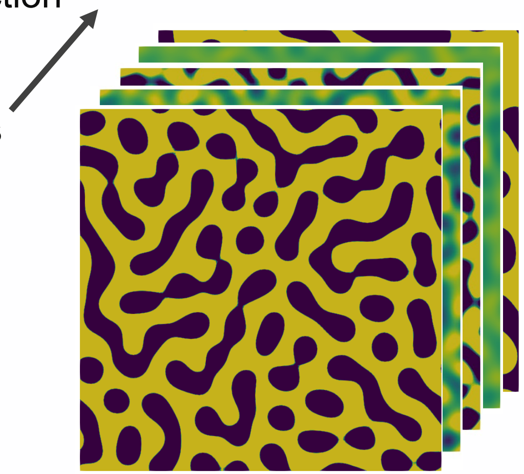
Localized Operator Inference: Offline Phase

Step 1 – Data collection & clustering

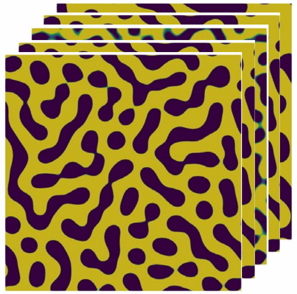
- Snapshot training data (e.g., from high-fidelity codes)

$$\mathbf{S} = \begin{bmatrix} | & | & & | \\ \mathbf{s}_0 & \mathbf{s}_1 & \cdots & \mathbf{s}_k \\ | & | & & | \end{bmatrix}, \dot{\mathbf{S}} = \begin{bmatrix} | & | & & | \\ \dot{\mathbf{s}}_0 & \dot{\mathbf{s}}_1 & \cdots & \dot{\mathbf{s}}_k \\ | & | & & | \end{bmatrix}, \mathbf{U} = \begin{bmatrix} | & | & & | \\ \boldsymbol{u}_0 & \boldsymbol{u}_1 & \cdots & \boldsymbol{u}_k \\ | & | & & | \end{bmatrix}$$

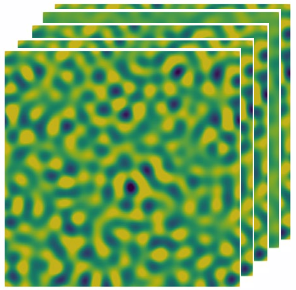
Snapshot collection across different timesteps and initial conditions



- Compute a global POD basis $\bar{\mathbf{V}} \in \mathbb{R}^{N\times q}$ (compression for clustering and classification)
- Low-dimensional data representation $\tilde{\mathbf{S}} = \bar{\mathbf{V}}^\top \mathbf{S}$:
- Partition training data into n_p snapshot clusters using unsupervised learning

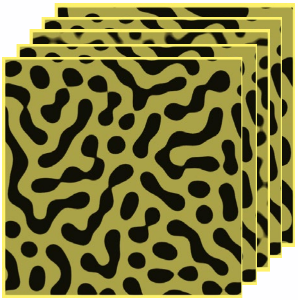


cluster 1



cluster 2

…



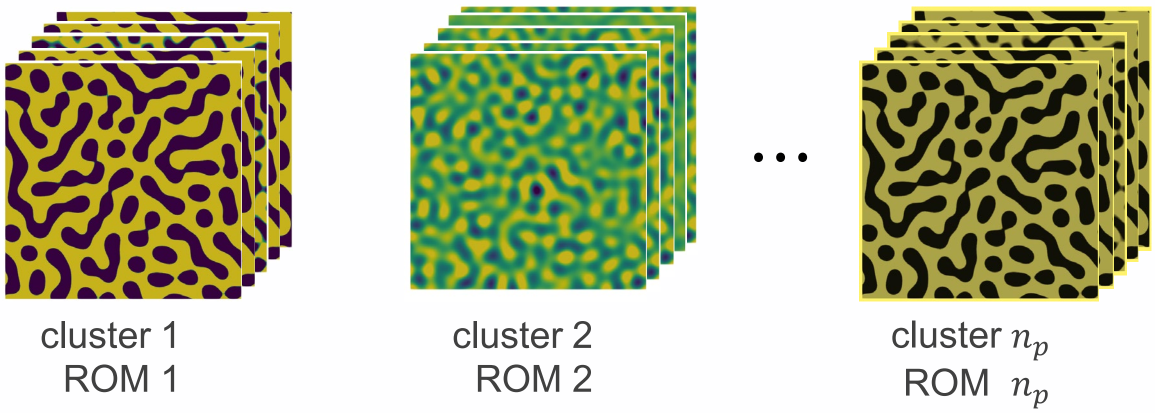
cluster n_p

Localized Operator Inference: Offline Phase

Step 2 – Train the classifier

- Nearest neighbor classifier maps from low-dimensional state $\tilde{\mathbf{S}}$ to cluster index

classifier: $\tilde{\mathbf{s}} \rightarrow \{1,2,\dots,n_p\}$



Step 3 – Learn n_p cluster-specific Operator Inference ROMs

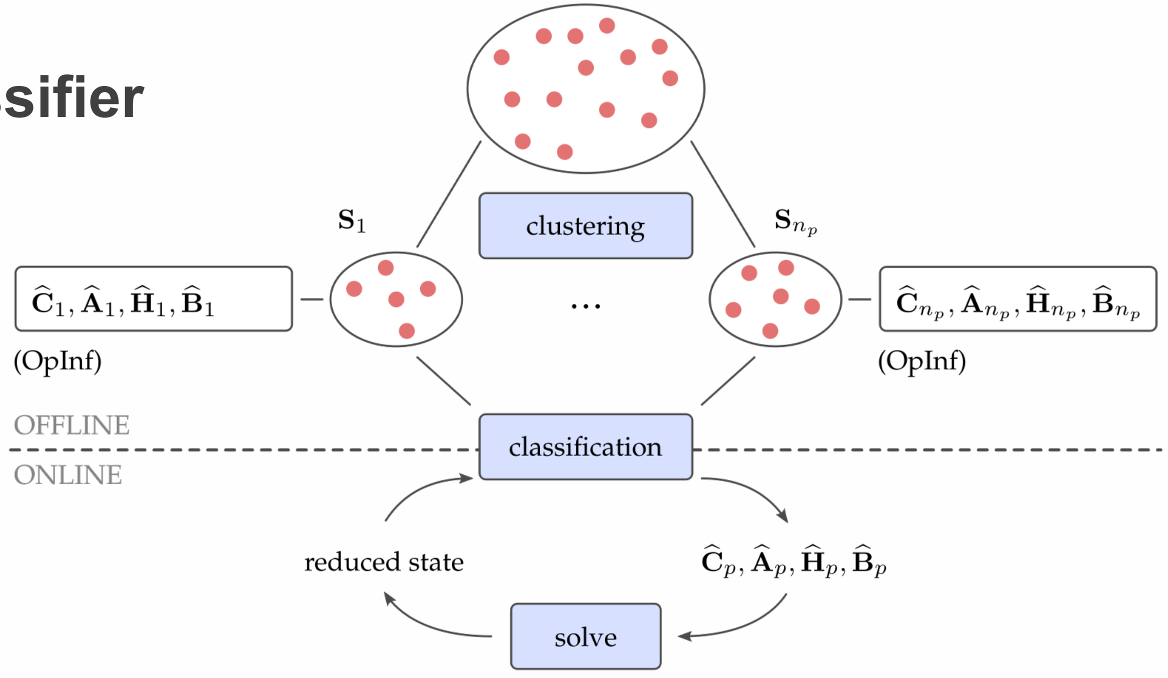
- Localized ROMs have cubic form (inherits structure of Cahn Hilliard):

$$\frac{\mathrm{d}}{\mathrm{dt}}\widehat{\mathbf{s}}_p(t) = \widehat{\mathbf{A}}_p\widehat{\mathbf{s}}_p(t) + \widehat{\mathbf{G}}_p\left(\widehat{\mathbf{s}}_p(t)\otimes\widehat{\mathbf{s}}_p(t)\otimes\widehat{\mathbf{s}}_p(t)\right)$$

- Solve linear least squares to infer localized operators $\widehat{\mathbf{A}}_p$ and $\widehat{\mathbf{G}}_p$

$$\underset{\widehat{\mathbf{A}}_p,\widehat{\mathbf{G}}_p}{\arg\min}\left(\left\|\widehat{\mathbf{A}}_p\widehat{\mathbf{S}}_p + \widehat{\mathbf{G}}_p\left(\widehat{\mathbf{S}}_p\odot\widehat{\mathbf{S}}_p\odot\widehat{\mathbf{S}}_p\right) - \dot{\widehat{\mathbf{S}}}_p\right\|_F^2 + \lambda_{1,p}\|\widehat{\mathbf{A}}_p\|_F^2 + \lambda_{2,p}\|\widehat{\mathbf{G}}_p\|_F^2\right)$$

Localized Operator Inference: Online Phase



Step 1 – Compute indicator and evaluate classifier

$$\tilde{\mathbf{s}} = \overline{\mathbf{V}}^\top \mathbf{V}_p \, \hat{\mathbf{s}}_p \in \mathbb{R}^q \;\; \rightarrow \;\; \{1, 2, \dots, n_p\}$$

Step 2 – ROM evaluation

- pth ROM:

$$\frac{\mathrm{d}}{\mathrm{dt}} \widehat{\mathbf{s}}_p(t) = \widehat{\mathbf{A}}_p \widehat{\mathbf{s}}_p(t) + \widehat{\mathbf{G}}_p \left(\widehat{\mathbf{s}}_p(t) \otimes \widehat{\mathbf{s}}_p(t) \otimes \widehat{\mathbf{s}}_p(t) \right)$$

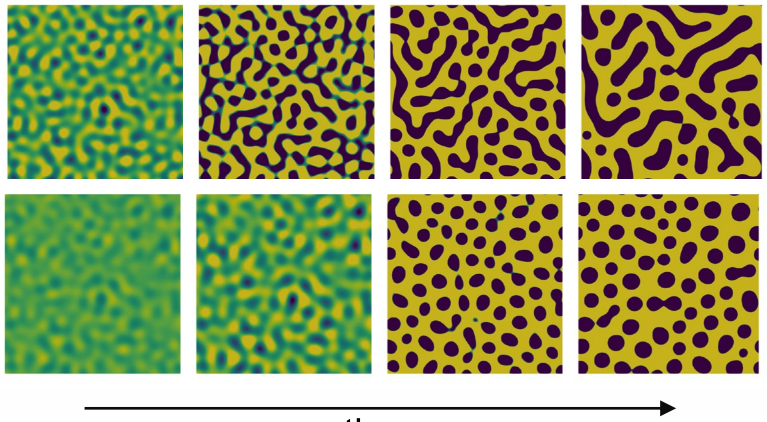
- When switching from cluster/ROM b to a, project the reduced state

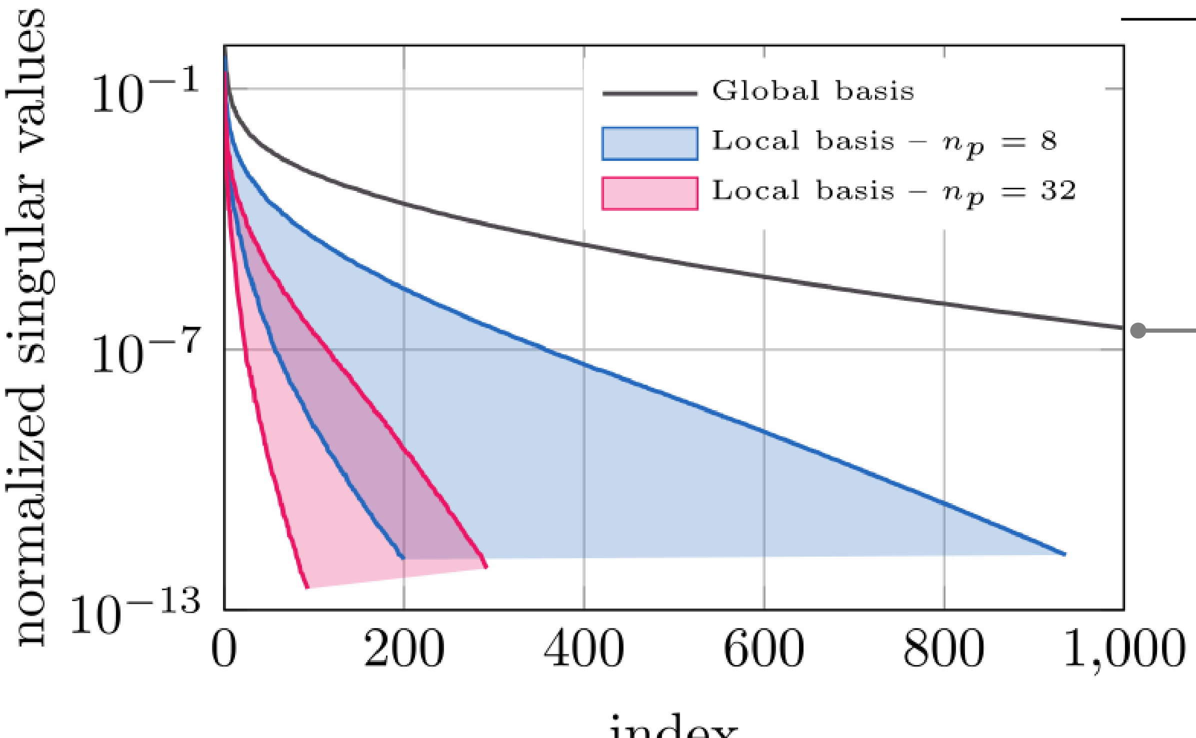
$$\hat{\mathbf{s}}_a = \mathbf{V}_a^\top \mathbf{V}_b \, \hat{\mathbf{s}}_b \in \mathbb{R}^{r_a}$$

Localization via clustering (unsupervised learning) is one way to mitigate slow singular value decay

$$\frac{\partial}{\partial t} s(\mathbf{x}, t) = M\nabla^2 \left(s^3(\mathbf{x}, t) - s(\mathbf{x}, t) - \ell \nabla^2 s(\mathbf{x}, t) \right)$$

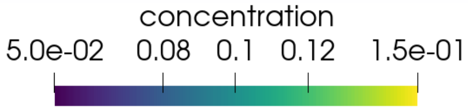
snapshots seeded with different initial conditions



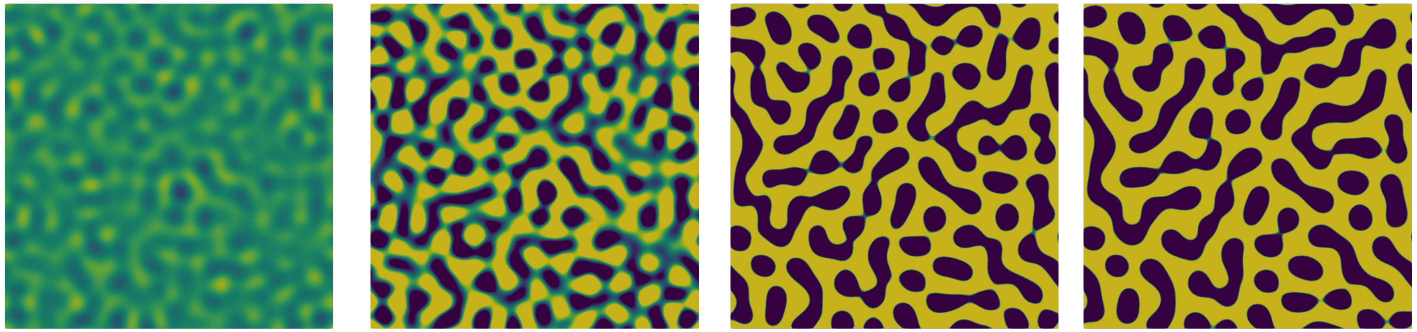


A global basis would require 10^2–10^3 modes

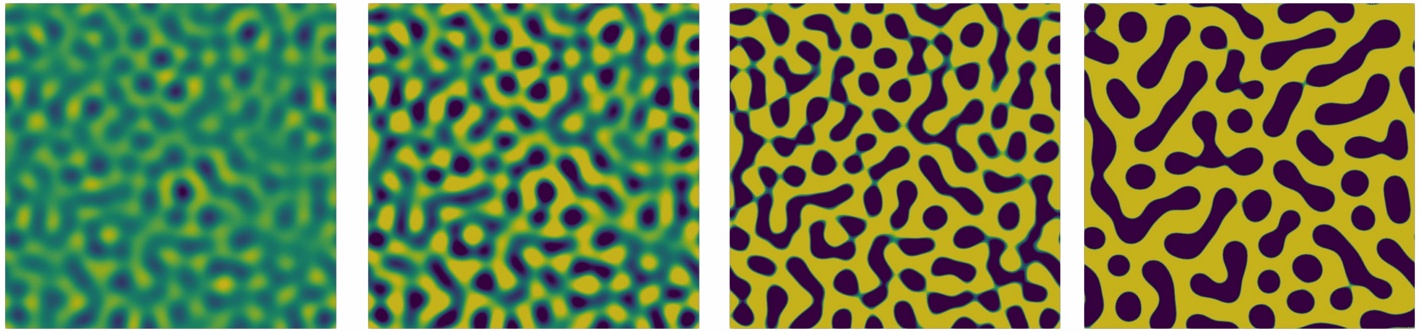
Reduced-order model performance

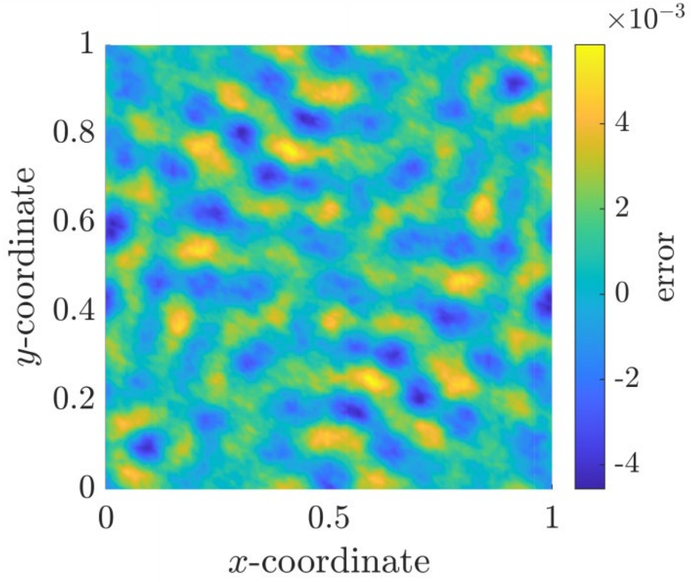


FOM $N = 16{,}384$

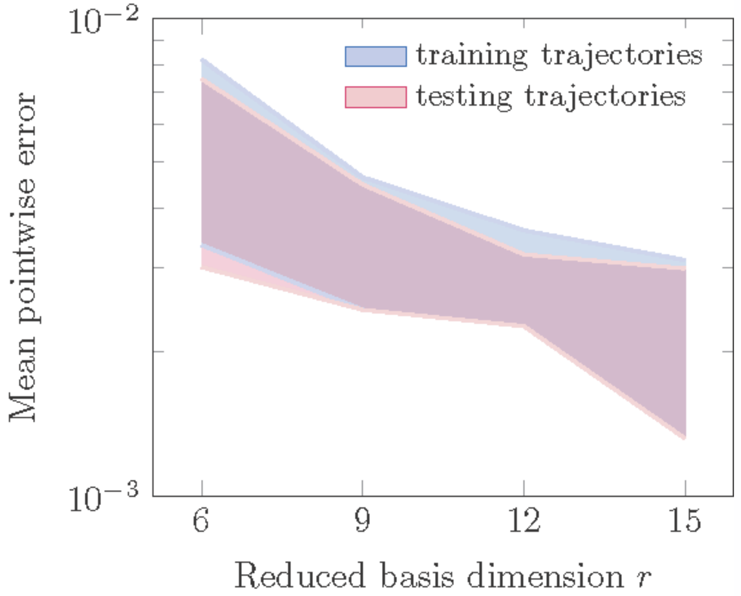


Localized OpInf ROM with 32 snapshot clusters, $r = 15$





Error in the autocorrelations



COMPUTATIONAL SCIENCE enables **AEROSPACE DESIGN**

1 **Learning from data**

The imperative of physics-based modeling & inverse theory

2 **Reduced-order modeling**

A critical enabler for accelerating predictive computations in support of engineering design

3 **Operator Inference**

Combining model reduction & machine learning to learn predictive reduced-order models

4 **Outlook**

Machine Learning → Scientific Machine Learning → Reduced Order Modeling

A range of tools for a range of use cases

Training data that cover the search space; need a fast efficient look-up table

Some training data but need to issue predictions beyond the training data

Trusted expensive code base; black box approximations (response surfaces) are sufficient

Trusted expensive code base; time and expertise to implement intrusive predictive reduced model

Challenges for **ENGINEERING DESIGN** in the age of **BIG DATA & BIG COMPUTE**

1. **Predictive modeling for complex systems at scale**
   Decisions demand a predictive window on the future

2. **Validation, verification & uncertainty quantification**
   Achieving the levels of reliability and robustness needed for certified high-consequence decision-making

3. **Data, models and decisions across multiple scales**
   Scalable algorithms for calibration, data assimilation, optimization, uncertainty quantification, planning & control

4. **Optimal sensing strategies**
   Digital twins, integrated sensor design, optimal experimental design (active learning), intelligent adaptive data acquisition

5. **Legacy codes and processes**
   Equipping our processes and our people with state-of-the-art computational science & computer science

Data-driven decisions

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

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