From reduced-order modeling to scientific machine learning

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

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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**
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
- Integrate sparse, heterogeneous, noisy & incomplete data
- Make predictions with quantified uncertainties
- Bring interpretability to results
- Support high-consequence decisions

BIG DECISIONS
THIS IS YOUR MACHINE LEARNING SYSTEM?

YUP! YOU POUR THE DATA INTO THIS BIG PILE OF LINEAR ALGEBRA, THEN COLLECT THE ANSWERS ON THE OTHER SIDE.

WHAT IF THE ANSWERS ARE WRONG?

JUST STIR THE PILE UNTIL THEY START LOOKING RIGHT.

https://xkcd.com/1838/
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", 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
Learning from data
The imperative of physics-based modeling & inverse theory

Reduced-order modeling
A critical enabler for accelerating predictive computations in support of engineering design

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

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
An Approximate Analytical Technique for Design Calculations

D. J. Fear and H. H. Mecky

The University of Scratton, Ohio

1. Introduction

The technique of simple, intuition, or in other words "guess and check," is to be found in every day practice. Many practical problems, from the design of an automobile to the operation of an engineering system, may be solved by this technique. The technique is simple, intuitive, and often yields results that are sufficiently accurate for practical purposes. However, when the problem becomes more complex, the technique may not be adequate.

2. Approximate Method

The approximate method is based on the principle of superposition, which states that the total response of a system to a given input is the sum of the responses to each input considered separately. This method is useful for analyzing systems that can be represented as a series of independent sub-systems.

3. Example

Consider the simple system shown in Figure 1. The system consists of a spring and a damper. The spring has a spring constant of 10 N/m and the damper has a damping coefficient of 5 Ns/m. The system is subjected to a step input of 10 N. Using the approximate method, the response of the system can be determined by calculating the response of each sub-system separately and then summing the results.

4. Conclusion

The approximate method is a useful tool for analyzing complex systems. It is simple to use and provides an accurate solution for many practical problems. However, the method may not be adequate for systems that cannot be represented as a series of independent sub-systems.
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**

\[
\dot{\hat{x}} = \hat{A}\hat{x} + \hat{B}u + \hat{H}(\hat{x} \otimes \hat{x})
\]

**Non-intrusive learning** by inferring reduced model operators \(\hat{A}, \hat{B}, \hat{H}\) 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

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

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

\[\sigma = C: \varepsilon\]

+ boundary conditions

+ initial conditions

---

**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 \(\sigma(x, y, t), \varepsilon(x, y, t), u(x, y, t), \ldots\)

---

A predictive window on the future
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Example: equations of linear elasticity

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\sigma = C: \varepsilon
\]

+ boundary conditions
+ initial conditions

A mathematical model of how solid objects deform, relating stress \(\sigma\), strain \(\varepsilon\), displacement \(u\), and loading \(F\).

A mathematical model solved with computational science

Discretize:
Spatially discretized computational fluid dynamic (CFD) model

\[
\dot{x} = Ax + Bu + f(x, u)
\]

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

E.g., nodal displacements

Example: equations of linear elasticity

Conservation of mass (\(\rho\)), momentum (\(\rho \vec{v}\)), energy (\(\rho c\)), chemical species (\(Y_{CH4}, Y_{O2}, Y_{CO2}, Y_{H2O}\)).
Full-order model (FOM) state \( x \in \mathbb{R}^N \)

Reduced-order model (ROM) state \( x_r \in \mathbb{R}^r \)

\[
\dot{x} = Ax + Bu
\]

Approximate \( x \approx Vx_r \)

\( V \in \mathbb{R}^{N \times r} \)

Residual: \( N \) eqs \( \gg r \) dof

\[
r = V\dot{x}_r - AVx_r - Bu
\]

Projecting a linear system

\[
W^T r = 0
\]

(Galerkin: \( W = V \))

\[
\dot{x}_r = A_r x_r + B_r u
\]

\[
A_r = V^T AV
\]

\[
B_r = V^T B
\]
Linear Model

FOM: \( \dot{x} = Ax + Bu \)

ROM: \( \dot{x}_r = A_r x_r + B_r u \)

Precompute the ROM matrices:

\[
A_r = V^T AV, \quad B_r = V^T B
\]

Quadratic Model

FOM: \( \dot{x} = Ax + H(x \otimes x) + Bu \)

ROM: \( \dot{x}_r = A_r x_r + H_r (x_r \otimes x_r) + B_r u \)

Precompute the ROM matrices and tensor:

\[
H_r = V^T H (V \otimes V)
\]

projection preserves structure \( \leftrightarrow \) structure embeds physical constraints
COMPUTATIONAL SCIENCE enables AEROSPACE DESIGN

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3. Operator Inference
   Combining model reduction & machine learning to learn predictive reduced-order models

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

\[
\min_0 \| D O - R \| 
\]

- **O**: low-dimensional operators that define the reduced model
- **D, 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
\[
\hat{x} = \hat{A}\hat{x} + \hat{B}u + \hat{H}(\hat{x} \otimes \hat{x})
\]

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

- Minimum residual formulation leads to linear least squares

\[
\min_{\hat{A}, \hat{B}, \hat{H}} \left\| \hat{X}^T \hat{A}^T + (\hat{X} \otimes \hat{X})^T \hat{H}^T + \hat{U}^T \hat{B}^T - \hat{X}^T \right\|
\]

- 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.
Rotating Detonation Engine (Farcas)

Phase-field modeling (Geelen)

Solidification in additive manufacturing (Khodabakhshi)

VAT Wing (Zastrow & Chaudhuri)
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

\[ \mathbf{S} = \begin{bmatrix} \mathbf{s}_0 & \mathbf{s}_1 & \cdots & \mathbf{s}_k \end{bmatrix} \]

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

normalized singular values

index
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

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

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

\[s_0 = 0.1\]

\[s_0 = 0.3\]

(a) \(t/T = 0.1\)  (b) \(t/T = 0.2\)  (c) \(t/T = 0.5\)  (d) \(t/T = 1\)
Localized Operator Inference: Offline Phase

Step 1 – Data collection & clustering

- Snapshot training data (e.g., from high-fidelity codes)
  \[ S = \begin{bmatrix} s_0 & s_1 & \cdots & s_k \end{bmatrix}, \dot{S} = \begin{bmatrix} \dot{s}_0 & \dot{s}_1 & \cdots & \dot{s}_k \end{bmatrix}, U = \begin{bmatrix} u_0 & u_1 & \cdots & u_k \end{bmatrix} \]

- Compute a global POD basis \( \bar{V} \in \mathbb{R}^{N \times q} \) (compression for clustering and classification)

- Low-dimensional data representation \( \hat{S} = \bar{V}^T S \)

- Partition training data into \( n_p \) snapshot clusters using unsupervised learning
Localized Operator Inference: Offline Phase

Step 2 – Train the classifier

- Nearest neighbor classifier maps from low-dimensional state $\tilde{s}$ to cluster index
  \[
  \text{classifier: } \tilde{s} \rightarrow \{1,2,\ldots,n_p\}
  \]

Step 3 – Learn $n_p$ cluster-specific Operator Inference ROMs

- Localized ROMs have cubic form (inherits structure of Cahn Hilliard):
  \[
  \frac{d}{dt} \hat{s}_p(t) = \hat{A}_p \hat{s}_p(t) + \hat{G}_p (\hat{s}_p(t) \otimes \hat{s}_p(t) \otimes \hat{s}_p(t))
  \]

- Solve linear least squares to infer localized operators $\hat{A}_p$ and $\hat{G}_p$
  \[
  \arg \min_{\hat{A}_p, \hat{G}_p} \left( \| \hat{A}_p \hat{s}_p + \hat{G}_p (\hat{s}_p \otimes \hat{s}_p \otimes \hat{s}_p) - \hat{s}_p \|_F^2 + \lambda_{1,p} \| \hat{A}_p \|_F^2 + \lambda_{2,p} \| \hat{G}_p \|_F^2 \right)
  \]
Localized Operator Inference: Online Phase

Step 1 – Compute indicator and evaluate classifier

\[ \tilde{s} = V_p^T V_p \hat{s}_p \in \mathbb{R}^q \rightarrow \{1, 2, \ldots, n_p\} \]

Step 2 – ROM evaluation

• \(\text{pth ROM:}\)

\[ \frac{d}{dt} \hat{s}_p(t) = \hat{A}_p \hat{s}_p(t) + \hat{G}_p (\hat{s}_p(t) \otimes \hat{s}_p(t) \otimes \hat{s}_p(t)) \]

• When switching from cluster/ROM \(b\) to \(a\), project the reduced state

\[ \hat{s}_a = V_a^T V_b \hat{s}_b \in \mathbb{R}^{r_a} \]
Localization via clustering (unsupervised learning) is one way to mitigate slow singular value decay

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

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

Localized OpInf ROM with 32 snapshot clusters, $r = 15$
Computational science enables aerospace design.

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4. **Outlook**
A range of tools for a range of use cases

- **Machine Learning**
  - Training data that cover the search space; need a fast efficient look-up table
  - Trusted expensive code base; black box approximations (response surfaces) are sufficient

- **Scientific Machine Learning**
  - Some training data but need to issue predictions beyond the training data

- **Reduced Order Modeling**
  - 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