

# **Predictive data science** for physical systems

From model reduction to scientific machine learning

**Professor Karen E. Willcox** 

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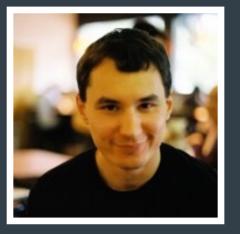


## Contributors









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Funding sources: US Air Force **Computational Math Program** (F. Fahroo); US Air Force **Center of Excellence on Rocket Combustion** (M. Birkan, F. Fahroo, D. Talley); SUTD-MIT **International Design Centre**  **1** Predictive Data Science

What & why

### 2 Lift and Learn

Projection-based model reduction as a lens through which to learn predictive models

## Outline

**3** Application example

Rocket engine combustion



#### **1 Predictive Data Science**

2 Lift & Learn

**3 Application Example** 

Predictive Data Science

4 Conclusions & Outlook

What and Why

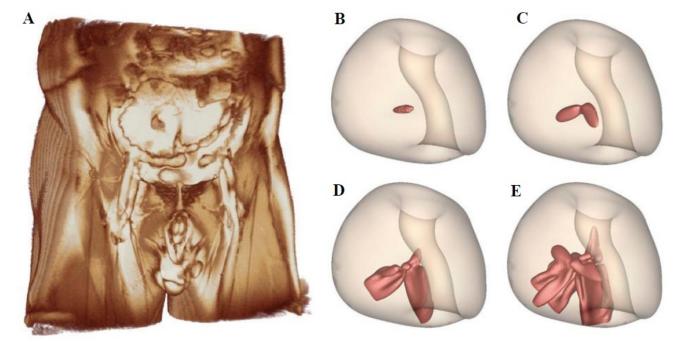


How do we harness the explosion of data to extract knowledge, insight and decisions?

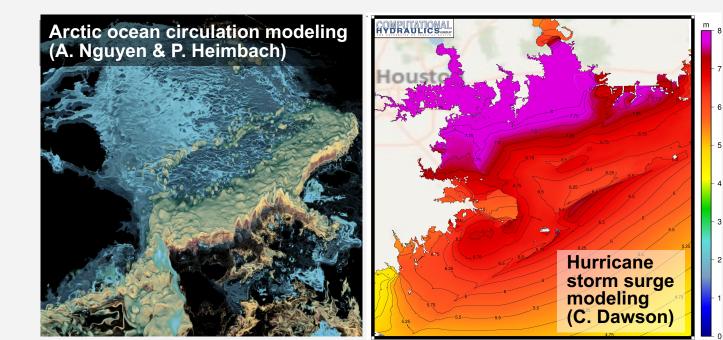
# **Big decisions** need more than just big data...

they need **big models** too

Inspired by Coveney, Dougherty, Highfield "Big data need big theory too"



Patient-specific prostate tumor modeling (T. Hughes)



## Big decisions need more than just big data...

Big decisions must incorporate the **predictive power**, **interpretability**, and **domain knowledge** of physics-based models



Predictive Data Science

a convergence of Data Science and Computational Science & Engineering

### Challenges

- 1 high-consequence applications are characterized by complex multiscale multiphysics dynamics
- 2 high (and even infinite) dimensional parameters
- 3 data are relatively sparse and expensive to acquire
- 4 uncertainty quantification in model inference and certified predictions in regimes beyond training data

## Learning from data through the lens of models...

```
dynamical systems
        uncertainty quantification
                              meshing methods
  Bayesian inference
                              finite volumes
                                             problems
large scale optimization
                     convergence analysis
     high performance computing
                                                         mage
                                 regularization
andomized
                projection-based
  nethods
      finite elements
                                            uction processing
partial differential
                      model reduction
     physics-based
      models
  boundary values
  data assimilation
                             approximation theory
  big data analysis
                                          error analysis
                 adjoints
                             importance sampling
                   low rank approximation
```

## Learning from data through the lens of models...

dynamical systems uncertainty quantification meshing methods **Bayesian** inference Inverse finite volumes large scale optimization convergence analysis high performance computing andomized regularization projection-based nethods finite elements model reduction processi physics-based models partial differential boundary values data assimilation approximation theory big data analysis error analysis adjoints importance sampling low rank approximation

1 Predictive Data Science

2 Lift & Learn

**3 Application Example** 

4 Conclusions & Outlook

# Lift & Learn

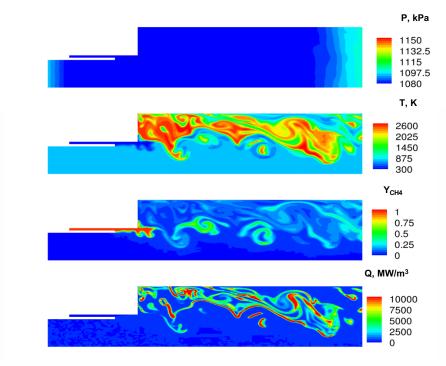
Projection-based model reduction as a lens through which to learn predictive models

# Lift & Learn: Ingredients

### 1. A physics-based model

Example: modeling combustion in a rocket engine Conservation of mass ( $\rho$ ), momentum ( $\rho \vec{w}$ ), energy (E), species ( $Y_{CH_4}$ ,  $Y_{O_2}$ ,  $Y_{CO_2}$ ,  $Y_{H_2O}$ )

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



- 2. Lens of **projection** to define a low-dimensional model
- 3. Variable transformations that expose polynomial structure in the model
- 4. Non-intrusive learning of the reduced model  $\rightarrow$  work with transformed variables



# **Projection-based model reduction**

Label: Solve PDEs to generate training data (<u>snapshots</u>)
 Identify structure: Compute a <u>low-dimensional basis</u>
 Train: <u>Project</u> PDE model onto the low-dimensional subspace

# Reduced models

Label
 Identify structure
 Train

 $\mathbf{E}_{r} = \mathbf{V}^{\top} \mathbf{E} \mathbf{V}$  $\mathbf{A}_{r} = \mathbf{V}^{\top} \mathbf{A} \mathbf{V}$  $\mathbf{H}_{r} = \mathbf{V}^{\top} \mathbf{H} (\mathbf{V} \otimes \mathbf{V})$  $\mathbf{B}_{r} = \mathbf{V}^{\top} \mathbf{B}$ 

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

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

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

Residual:  $N \text{ eqs} \gg r \text{ dof}$  $r = EV\dot{x}_r - AVx_r - Bu$ 

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

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

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

# Linear Model

FOM:  $E\dot{x} = Ax + Bu$ 

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

Precompute the ROM matrices:

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

# **Quadratic Model**

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

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

Precompute the ROM matrices and tensor:

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

projection preserves structure  $\leftrightarrow$  structure embeds physical constraints

#### **Machine learning**

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

### **Reduced-order modeling**

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

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

Model reduction methods have grown from CSE, with a focus on *reducing* high-dimensional models that arise from physics-based modeling, whereas machine learning has grown from CS, with a focus on *creating* low-dimensional models from black-box data streams. Yet recent years have seen an increased blending of the two perspectives and a recognition of the associated opportunities. [Swischuk et al., *Computers & Fluids*, 2018]

$$\begin{bmatrix} \frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \rho u^{2} + p \\ \rho u^{2} + p \end{pmatrix} = 0 \\ E = \frac{p}{\gamma - 1} \begin{bmatrix} \frac{\partial}{\partial t} \begin{pmatrix} \rho \\ u \\ p \end{pmatrix} + \begin{pmatrix} \rho \frac{\partial u}{\partial x} + u \frac{\partial \rho}{\partial x} \\ u \frac{\partial i}{\partial x} \\ \gamma p \frac{\partial}{\partial t} \frac{\partial}{\partial t} \begin{pmatrix} u \\ p \end{pmatrix} + \begin{pmatrix} u \frac{\partial u}{\partial x} + q \frac{\partial p}{\partial x} \\ \gamma p \frac{\partial}{\partial t} \frac{\partial}{\partial t} \begin{pmatrix} u \\ p \end{pmatrix} \\ \gamma p \frac{\partial}{\partial t} \frac{\partial}{\partial t} \begin{pmatrix} u \\ p \end{pmatrix} + \begin{pmatrix} u \frac{\partial u}{\partial x} + q \frac{\partial p}{\partial x} \\ \gamma p \frac{\partial u}{\partial x} + u \frac{\partial p}{\partial x} \\ q \frac{\partial u}{\partial x} + u \frac{\partial q}{\partial x} \end{pmatrix} = 0$$

## Variable Transformations & Lifting

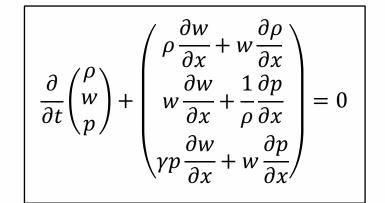
The physical governing equations reveal variable transformations and manipulations that expose polynomial structure

There are multiple ways to write the Euler equations

Different choices of variables leads to different *structure* in the discretized system  $\rightarrow$  *lifting* 

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho w \\ E \end{pmatrix} + \frac{\partial}{\partial z} \begin{pmatrix} \rho w \\ \rho w^2 + p \\ (E+p)w \end{pmatrix} = 0$$
$$E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho w^2$$

conservative variables mass, momentum, energy

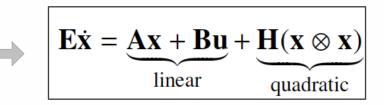


primitive variables mass, velocity, pressure

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

$$\frac{\partial}{\partial t} \binom{w}{p}_{q} + \binom{w \frac{\partial w}{\partial x} + q \frac{\partial p}{\partial x}}{p \frac{\partial w}{\partial x} + w \frac{\partial p}{\partial x}} = 0$$
$$\frac{\partial w}{q \frac{\partial w}{\partial x} + w \frac{\partial q}{\partial x}}$$

specific volume variables



transformed system has linear-quadratic structure

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

# Simple example

Lifting a nonlinear (quartic) ODE to quadratic-bilinear form

Can either lift to a system of ODEs or to a system of DAEs Consider the quartic system

Introduce auxiliary variables:

Chain rule:

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

Need additional variable to make auxiliary dynamics quadratic:  $w_3 = xw_1$   $\dot{w}_3 = \dot{x}w_1 + x\dot{w}_1$   $= w_1w_2 + w_1u + 2w_1w_2 + 2w_1u$  **QB-ODE**  $\dot{x} = w_2 + u$  **QB-DAE** 

$$\dot{w}_1 = 2xw_2 + 2xu$$
$$\dot{w}_2 = 4w_2w_3 + 4w_3u$$
$$\dot{w}_3 = 3w_1w_2 + 3w_1u$$

QB-DAE $\dot{x} = w_1^2 + u$  $0 = w_1 - x^2$ 

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

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

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

original equations

Many different forms of nonlinear equations can be lifted to polynomial form

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

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

$$\dot{w}_1 = \gamma \ w_6 \left[\frac{1}{Pe}\psi_{ss} - \psi_s\right] + \gamma \mathcal{B}\mathcal{D} \ w_4w_6$$

$$\dot{w}_2 = -2 \ w_5 \odot \left[\frac{1}{Pe}\psi_{ss} - \psi_s\right] - 2\mathcal{B}\mathcal{D} \ w_4w_5$$

$$\dot{w}_3 = -w_2 \odot \left[\frac{1}{Pe}\psi_{ss} - \psi_s\right] - \mathcal{B}\mathcal{D} \ w_2w_4$$

$$0 = w_4 - w_1\psi$$

$$0 = w_5 - w_2w_3$$

$$0 = w_6 - w_1w_2$$
quadratic-bilinear  
lifted equations

# **Operator inference**

Non-intrusive learning of the reduced models from simulation snapshot data

Given state data, learn the system

In principle could learn a large, sparse system e.g., Schaeffer, Tran & Ward, 2017

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

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

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

Find the operators **A**, **B**, **E**, **H** by solving the least squares problem:

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

Given *reduced* state data, learn the *reduced* model

### **Operator Inference**

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

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

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

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

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

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

Under certain conditions, recovers the intrusive POD reduced model

# Lift & Learn

Variable transformations to expose structure+ non-intrusive learning that frees us to choose our variables

Using only snapshot data from the high-fidelity model (non-intrusive) but learning the POD reduced model Lift & Learn [Qian, Kramer, Peherstorfer & W., 2019]

 Generate full state trajectories (snapshots) (from high-fidelity simulation)

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

Using only snapshot data from the high-fidelity model (non-intrusive) but learning the POD reduced model Lift & Learn [Qian, Kramer, Peherstorfer & W., 2019]

- Generate full state trajectories (snapshots) (from high-fidelity simulation)
- 2. Transform snapshot data to get lifted snapshots (analyze the PDEs to expose system polynomial structure)

$$X_{orig} \rightarrow X$$
  $\dot{X}_{orig} \rightarrow \dot{X}$ 

Using only snapshot data from the high-fidelity model (non-intrusive) but learning the POD reduced model

#### Lift & Learn [Qian, Kramer, Peherstorfer & W., 2019]

- Generate full state trajectories (snapshots) (from high-fidelity simulation)
- 2. Transform snapshot data to get lifted snapshots
- 3. Compute POD basis from lifted trajectories

 $\mathbf{X} = \mathbf{V} \, \boldsymbol{\Sigma} \, \mathbf{W}^{\top}$ 

Using only snapshot data from the high-fidelity model (non-intrusive) but learning the POD reduced model

#### Lift & Learn [Qian, Kramer, Peherstorfer & W., 2019]

- Generate full state trajectories (snapshots) (from high-fidelity simulation)
- 2. Transform snapshot data to get lifted snapshots
- 3. Compute POD basis from lifted trajectories
- 4. Project lifted trajectories onto POD basis, to obtain trajectories in low-dimensional POD coordinate space

$$\widehat{\mathbf{X}} = \mathbf{V}^\top \mathbf{X}$$

Using only snapshot data from the high-fidelity model (non-intrusive) but learning the POD reduced model

#### Lift & Learn [Qian, Kramer, Peherstorfer & W., 2019]

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

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

Using only snapshot data from the high-fidelity model (non-intrusive) but learning the POD reduced model

#### Lift & Learn [Qian, Kramer, Peherstorfer & W., 2019]

- Generate full state trajectories (snapshots) (from high-fidelity simulation)
- 2. Transform snapshot data to get lifted snapshots
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Under certain conditions, recovers the intrusive POD reduced model

→ convenience of black-box learning + rigor of projection-based reduction + structure imposed by physics 1 Predictive Data Science

2 Lift & Learn

**3 Application Example** 

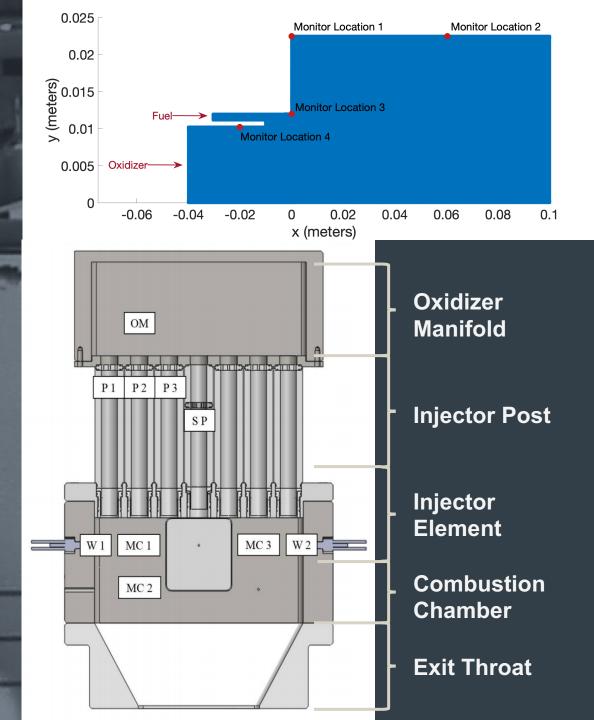
4 Conclusions & Outlook

# Rocket Engine Combustion

Lift & Learn reduced models for a complex Air Force combustion problem

## Modeling a single injector of a rocket engine combustor

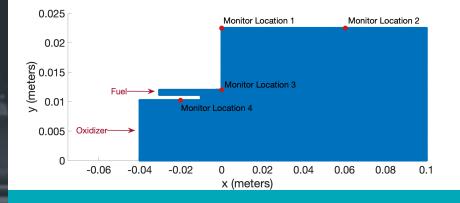
- Spatial domain discretized into 38,523 cells
- Pressure monitored at 4 locations
- Oxidizer input: 0.37  $\frac{\text{kg}}{\text{s}}$  of 42%  $\text{O}_2$  / 58%  $\text{H}_2\text{O}$
- Fuel input: 5.0  $\frac{\text{kg}}{\text{s}}$  of CH<sub>4</sub>
- Governing equations: conservation of mass, momentum, energy, species
- Forced by a back pressure boundary condition at exit throat



# Modeling a single injector of a rocket engine combustor

#### Training data

- 1ms of full state solutions generated using Air Force GEMS code (~200 hours CPU time)
- Timestep  $\Delta t = 10^{-7}$ s; 10,000 total snapshots
- Variables used for learning ROMs  $\mathbf{x} = \begin{bmatrix} \mathbf{p} & \mathbf{u} & \mathbf{v} & 1/\rho & Y_{CH_4} & Y_{O_2} & Y_{CO_2} & Y_{H_2O} \end{bmatrix}$ makes many (but not all) terms in governing equations quadratic
- Snapshot matrix  $\mathbf{X} \in \mathbb{R}^{308,184 \times 10,000}$

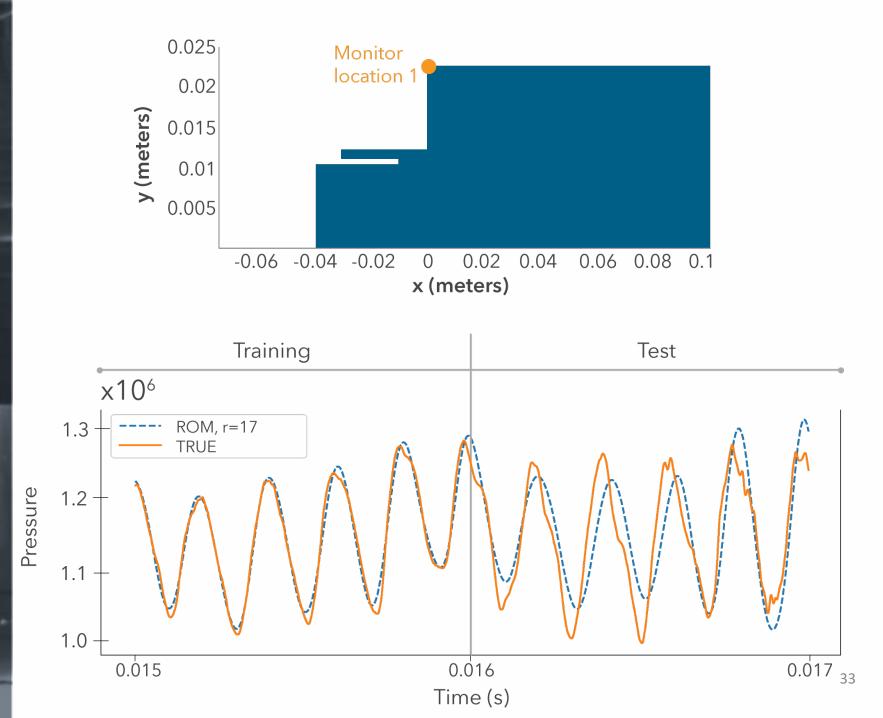


#### **Test data**

Additional 1 ms of data at monitor locations (10,000 timesteps) Performance of learned quadratic ROM

Pressure time traces at monitor location 1

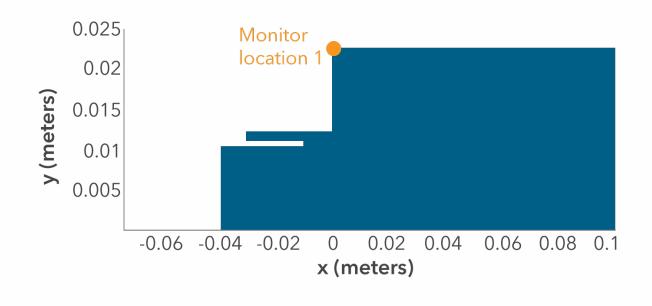
Basis size r = 17

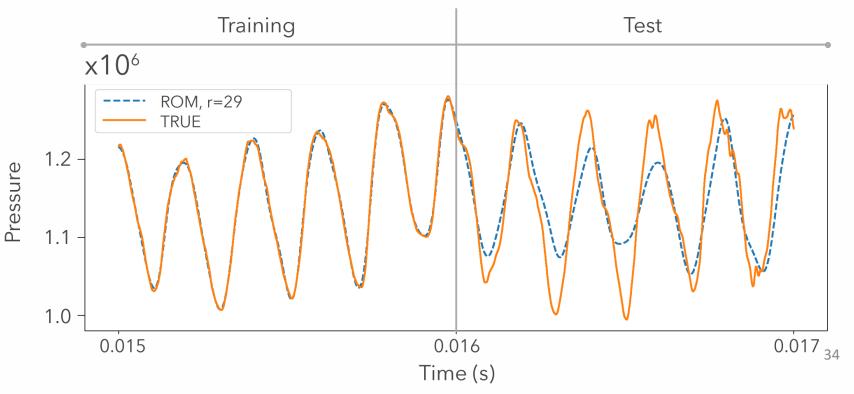


Performance of learned quadratic ROM

Pressure time traces at monitor location 1

Basis size r = 29





True

#### Pressure

0.03

0.02

0.01

0

0

#### Temperature

0.1

К 2500

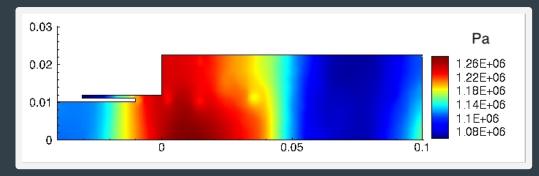
2000

1500

1000

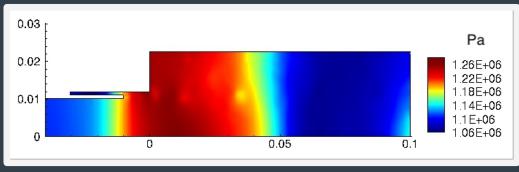
500

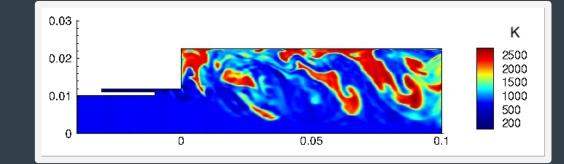
200



## Predicted

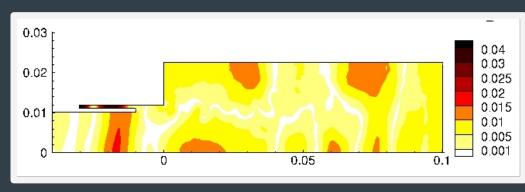
r = 29 POD modes

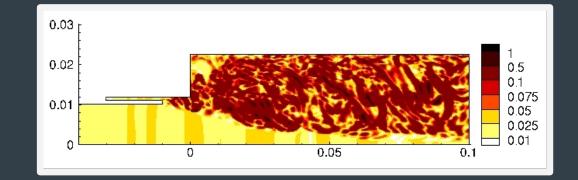




0.05

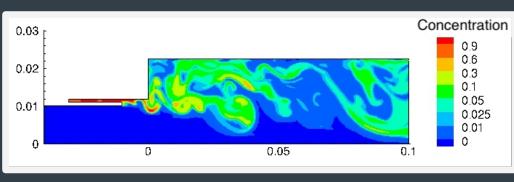
#### **Relative error**





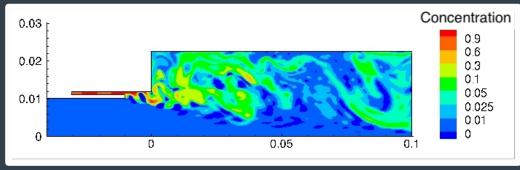
True

 $CH_4$ 

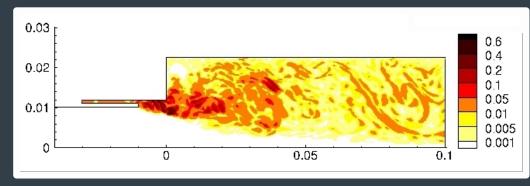


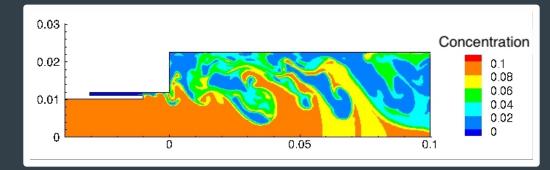
### Predicted

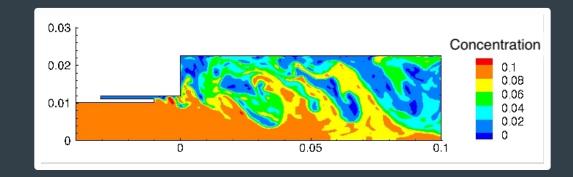
r = 29 POD modes

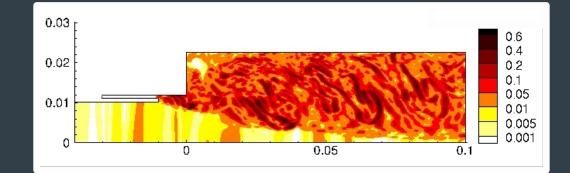


#### Normalized absolute error









**O**<sub>2</sub>

1 Predictive Data Science

2 Concrete Example

**3** Application Example

4 Conclusions & Outlook

# Conclusions & Outlook

The future of Predictive Data Science

#### **Data Science**

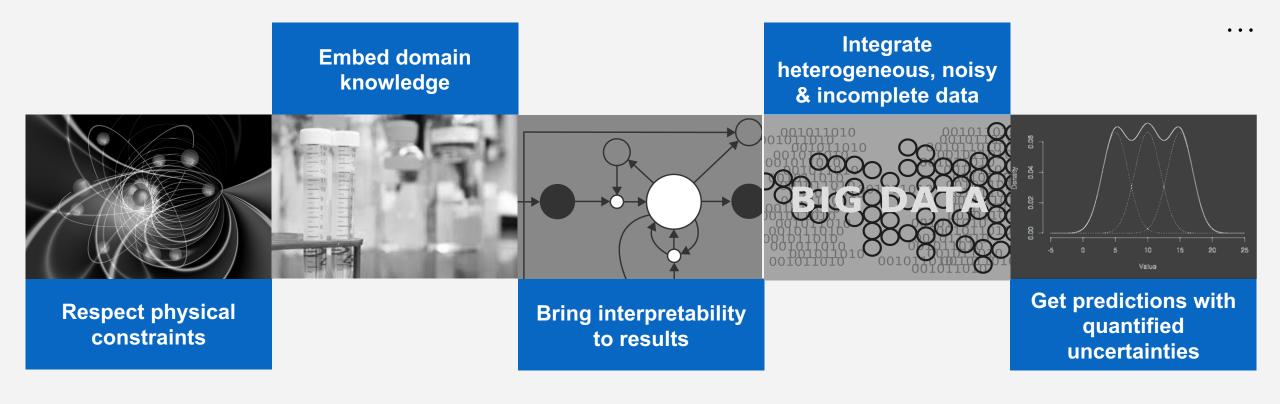
Computational Science & Engineering

# Predictive Data Science

Revolutionizing decision-making for high-consequence applications in science, engineering & medicine

# **Predictive Data Science**

Learning from data through the lens of models is a way to exploit structure in an otherwise intractable problem.



# Predictive Data Science

### Embedding domain knowledge

1

3

Learning from data through the lens of models

2

4

Needs interdisciplinary research & education at the interfaces

Principled approximations that exploit low-dimensional structure

Explicit modeling & treatment of uncertainty

# **Data-driven** decisions

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

## **KIWI.ODEN.UTEXAS.EDU**



# Our papers on this topic

- 1. Peherstorfer, B. and Willcox, K., Data-driven operator inference for nonintrusive projection-based model reduction, *Computer Methods in Applied Mechanics and Engineering*, Vol. 306, pp. 196-215, 2016.
- Kramer, B. and Willcox, K., Nonlinear model order reduction via lifting transformations and proper orthogonal decomposition, *AIAA Journal*, Vol. 57 No. 6, pp. 2297-2307, 2019.
- 3. Qian, E., Kramer, B., Marques, A. and Willcox, K., Transform & Learn: A datadriven approach to nonlinear model reduction. In Proceedings of AIAA Aviation Forum & Exhibition, Dallas, TX, June 2019.