# Model Order Reduction for Multi-scale, Multi-physics Problems

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# Speakers

The goal of this workshop is two-fold:

a) Introduce data-driven and reduced order modeling, and

b) Present leading-edge research performed under the Air Force Center of Excellence project (U.Michigan/UT-Austin/NYU/Purdue/Kansas) to AFRL and various DoD stakeholders.

The first day will be about foundational linear algebra.

The second day will introduce basics of data-driven & reduced order modeling.

The third day will cover advanced topics.

**Lecture notes** will be provided for part of the material.

**Day 1 (Tuesday, Aug 29)**

1:00 PM Welcome, Introductory remarks

1:30PM – 4:00PM Background in Numerical Linear algebra & Machine learning - **Duraisamy (UM)**

4:00PM – 4:30PM Discussion

**Day 2 (Wednesday, Aug 30)**

9:30 – 10:30AM Projection-based reduced order modeling - basics - **Peherstorfer (NYU)**

10:45AM – 12:00PM Linear Model Order Reduction - **Rezaian (UM)**

1:30 – 2:45PM Learning dynamical systems from data – basics – **Farcas (UT)**

3:00 – 4:30PM Adaptivity in Reduced Order models - **Peherstorfer (NYU)**

4:30 – 5:00 PM ROM Demo (1D test code: https://github.com/cwentland0/perform) - **Rezaian (UM)**

**Day 3 (Thursday, Aug 31)**

9:30 – 10:45AM Robust & Scalable Reduced Order Models - **Duraisamy (UM)**

11:00AM – 12:15PM Non-intrusive Reduced Order Models: application to large-scale systems - **Farcas (UT)**

1:30 – 2:15 PM Adaptive Reduced Order models for chaotic multi-scale problems - **Huang (KU)**

2:30 - 3:30 PM Component-based ROMs (ROM Networks) - **Huang (KU)**

3:30 – 4:30 PM Discussion

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# Resources

https://caslab.engin.umich.edu/teaching

1. PERFORM (Prototyping environment for reacting flow order reduction methods : code)
2. PERFORM (Prototyping environment for reacting flow order reduction methods : doc)

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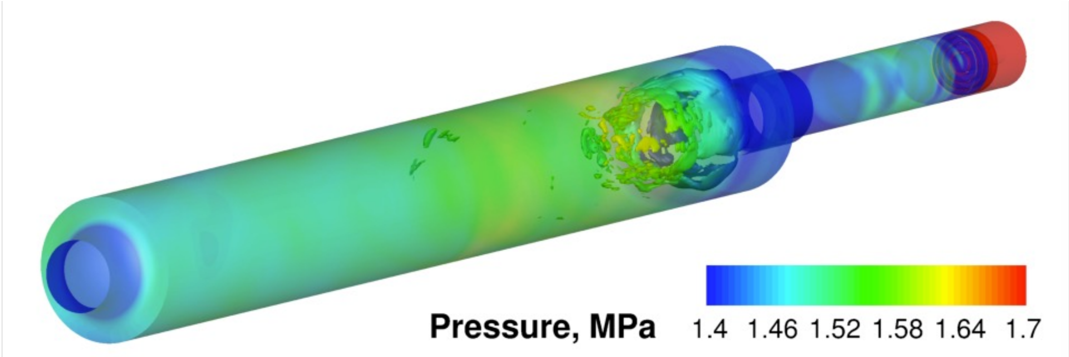
# Motivation: What does it take to perform a ”reasonably” high fidelity simulation of a single rocket injector ?




Purdue Single element Rocket combustor :
50 milli-seconds of simulation time = 25 exaflop of computing resources
= 1 month on 1000 core cluster

1 Merlin engine:
50 milli-seconds of simulation time = 2500 exaflop of computing resources
= 70 hours on fastest computer in the world*
= 10 months on 10,000 core cluster

*$200k electricity cost / $4.4M compute cost (cloud)

# Landscape of Modeling

High Fidelity Models
Pro: Predictivity, Math/physical consistency
Con: Cost

Reduced Order Models:
Pro: Math/physical consistency
Con: Robustness & Generalization

Reduced Fidelity Models:
Pro: Insight, efficiency
Con: Limited Generalization

## Projection-based Reduced Order Models

Convection + diffusion + source

$$\frac{\mathrm{d}\mathbf{q}(t,\mathbf{p})}{\mathrm{d}t} = \mathbf{f}(\mathbf{q}(t,\mathbf{p})) \quad ; \quad \mathbf{q} \in \mathbb{R}^n$$

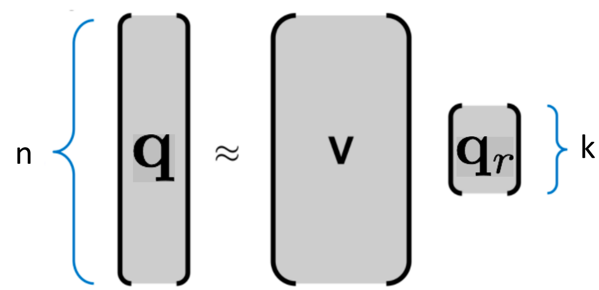
**HFM** n ~ $O(10^9)$

$$\frac{\mathrm{d}\mathbf{q}_r(t,\mathbf{p})}{\mathrm{d}t} = \mathbf{f}_r(\mathbf{q}_r(t,\mathbf{p})) \quad ; \quad \mathbf{q}_r \in \mathbb{R}^k$$

**ROM** k ~ $O(10^3)$

$$\mathbf{q}(t,\mathbf{p}) \approx \mathbf{V}\mathbf{q}_r(t,\mathbf{p}) \quad ; \quad \mathbf{V} \in \mathbb{R}^{n\times k}$$

**Reduced Basis approximation** **Basis**




Basis V obtained from a knowledge of the solution

Goal is to ensure accuracy when k << n & efficiently evaluate $f_r$

## Some Model Order Reduction methods (More mature topics)

• **Proper orthogonal decomposition** (POD) *(Lumley, 1967; Sirovich, 1981; Berkooz, 1991; Deane et al. 1991; Holmes et al. 1996)*
  – use data to generate empirical eigenfunctions – time- and frequency-domain methods

• **Krylov-subspace** methods *(Gallivan, Grimme, & van Dooren, 1994; Feldmann & Freund, 1995; Grimme, 1997, Gugercin et al., 2008)*
  – rational interpolation

• **Balanced truncation** *(Moore, 1981; Sorensen & Antoulas, 2002; Li & White, 2002)*
  – guaranteed stability and error bound for LTI systems
  – close connection between POD and balanced truncation

• **Reduced basis** methods *(Noor & Peters, 1980; Patera & Rozza, 2007)*
  – strong focus on error estimation for specific PDEs

• **Eigensystem realization algorithm** (ERA) *(Juang & Pappa, 1985)*, **Dynamic mode decomposition** (DMD) *(Schmid, 2010)*, **Loewner** model reduction *(Mayo & Antoulas, 2007)*
  – data-driven, non-intrusive

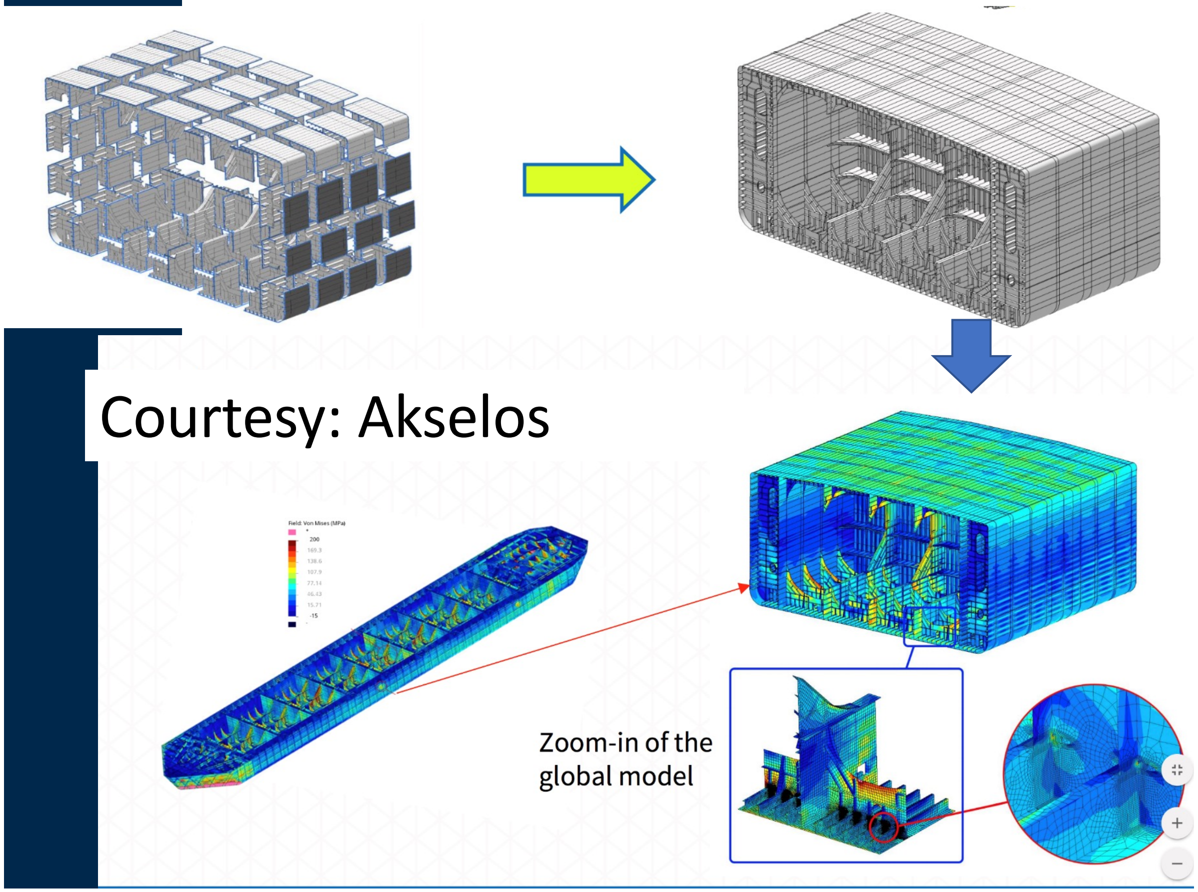
**Reduced Order Models**

Reduced order models have been used successfully in many fields ➔ Mostly in linear / mildly non-linear problems, elliptic problems, highly viscous problems

Courtesy: Akselos

## Reduced Order Models

Reduced order models have been used successfully in many fields ➔ Mostly in linear / mildly non-linear problems, elliptic problems, highly viscous problems



# Model Order Reduction

Volume 1: System- and Data-Driven Methods and Algorithms

Edited by
Peter Benner, Stefano Grivet-Talocia, Alfio Quarteroni,
Gianluigi Rozza, Wil Schilders, and Luís Miguel Silveira

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## Some Notable advances in ROMs of 'Complex' Fluid flows

- ROMs based on POD , Balanced POD, etc. (Rowley, Willcox, etc.. Mid 2000s)
- Empirical Interpolation, Discrete Empirical Interpolation (Maday, Sorenson, etc.. Mid-late 2000s)
- Closures, Stabilization (Cordier, Illescu, Tezaur, Duraisamy, etc.. Mid 2000s – late 2010s)
- Least Squares Petrov Galerkin, GNAT (Farhat, Carlberg, etc.. Late 2000s to mid 2010s)
- Local bases, Feature tracking (Zahr etc.. Mid 2010s)
- Adaptive bases (Perherstorfer, etc… late 2010s, Zahr, Huang, etc.)
- Non-intrusive ROMs (Willcox, Hesthaven, etc.. Late 2010s)

# Motivation : Predictive ROMs for Extremely stiff/Non-linear Transport problems

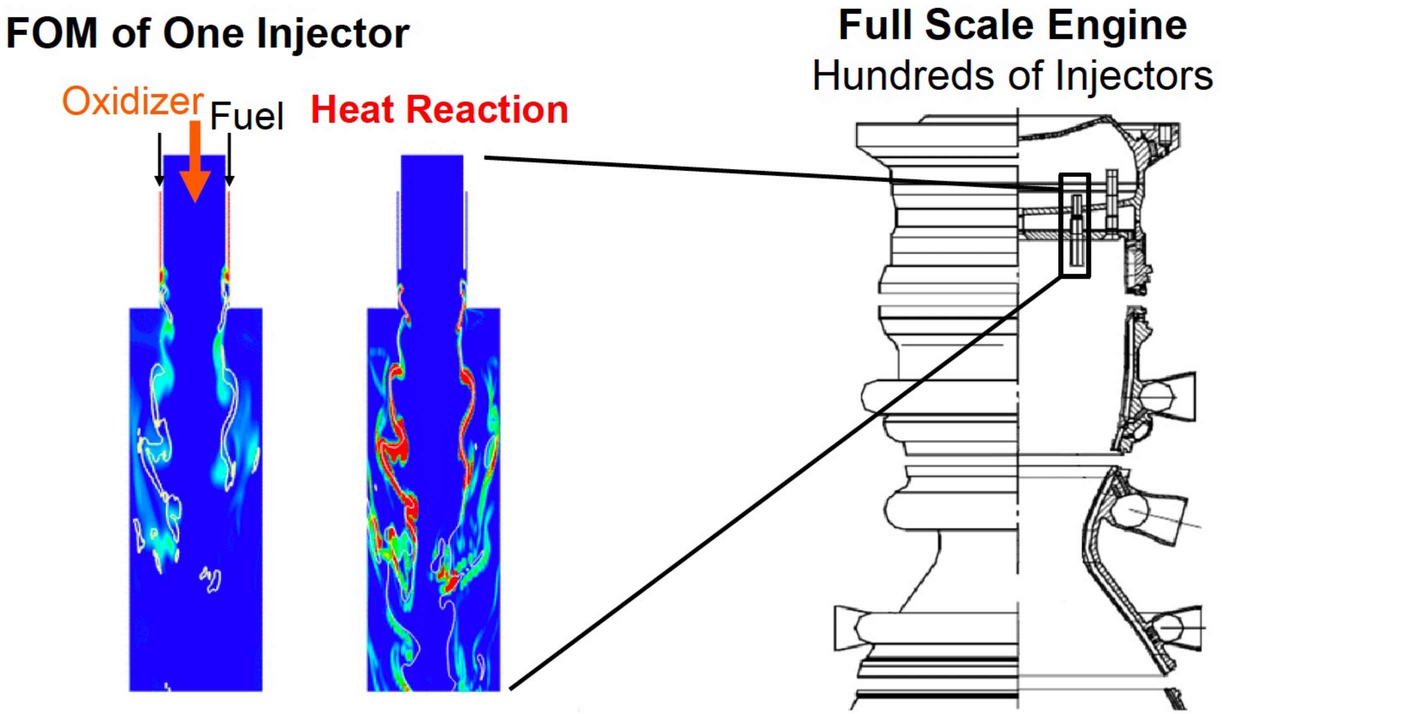
Introduction

SP-LSVT ROMs
- Formulation
- Results

Adaptive Basis
- Formulation
- Results

ROM Networks
- Formulation
- Results

Summary




10M cells, 1,000 processors, ~1 month

>>100M cells, 10,000 processors, > 12 months

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Introduction

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Summary


# Multi-scale, Multi-physics, Complexity : An Example

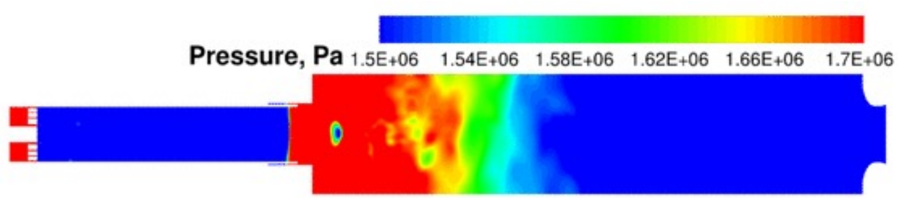
- Non-linear, Multi-scale multi-physics interactions : acoustics, flow & reaction
- Flow – Large coherent structures + small shear layer dynamics
- Reaction – Highly intensive, distributed & intermittent thin flame
- High sensitivity to parameter changes

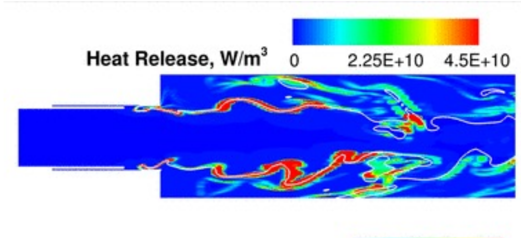
$$\frac{\partial Q}{\partial t} + \frac{\partial F_i}{\partial x_i} + \frac{\partial F_{v,i}}{\partial x_i} = H$$

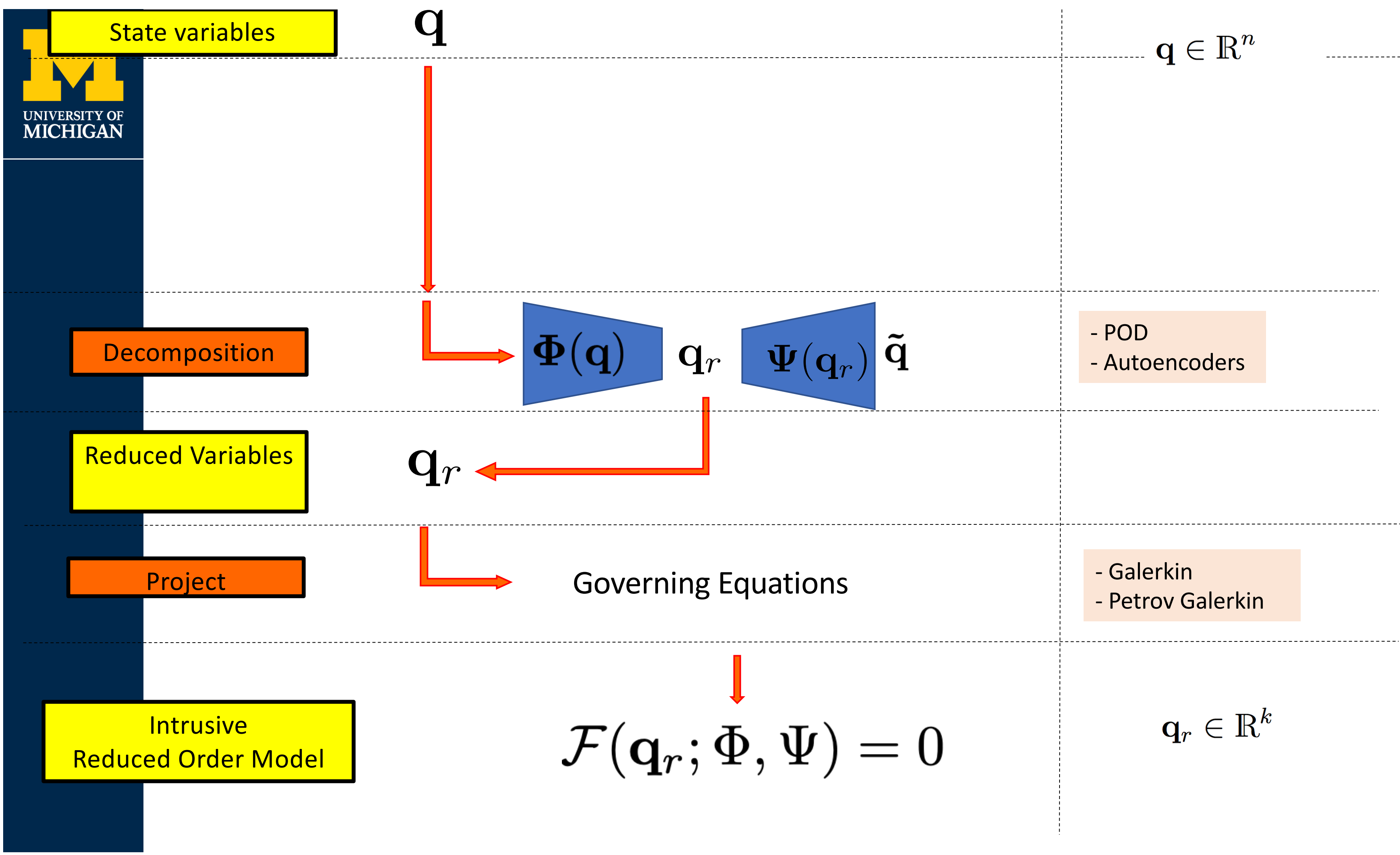
$$Q = \begin{pmatrix} \rho \\ \rho u_i \\ \rho h^0 - p \\ \rho Y_l \end{pmatrix}, \quad F_i = \begin{pmatrix} \rho u_i \\ \rho u_i u_j \\ \rho u_i h^0 \\ \rho u_i Y_l \end{pmatrix}, \quad F_{v,i} = \begin{pmatrix} 0 \\ \tau_{ij} \\ u_j \tau_{ji} + q_i \\ \rho V_{i,l} Y_l \end{pmatrix}, \quad H = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \dot{\omega}_l \end{pmatrix}$$

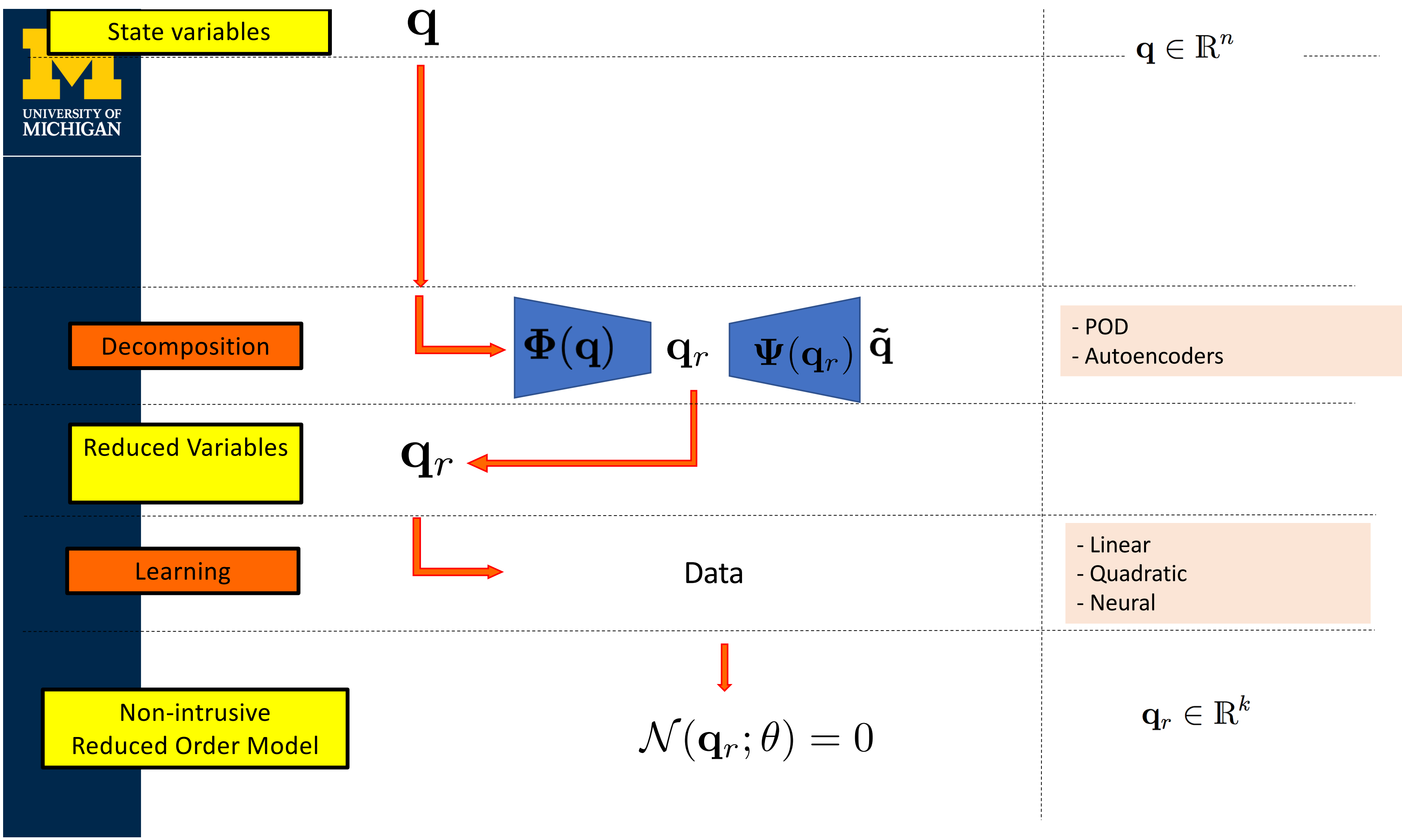
**Highly nonlinear and stiff source term :**

$$e.g., \ \dot{\omega}_1 = \frac{\rho Y_1}{M_1} A T^b \exp\left(\frac{-E_a}{R_u T}\right) [\frac{\rho Y_1}{M_1}]^{0.2} [\frac{\rho Y_2}{M_2}]^{1.3}$$




State variables
$\mathbf{q}$
$\mathbf{q} \in \mathbb{R}^n$
Decomposition
$\Phi(\mathbf{q})$
$\mathbf{q}_r$
$\Psi(\mathbf{q}_r)$
$\tilde{\mathbf{q}}$
- POD
- Autoencoders
Reduced Variables
$\mathbf{q}_r$
Project
Governing Equations
- Galerkin
- Petrov Galerkin
Intrusive Reduced Order Model
$\mathcal{F}(\mathbf{q}_r; \Phi, \Psi) = 0$
$\mathbf{q}_r \in \mathbb{R}^k$



State variables
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Decomposition
$\mathbf{\Phi}(\mathbf{q})$
$\mathbf{q}_r$
$\mathbf{\Psi}(\mathbf{q}_r)$
$\tilde{\mathbf{q}}$
- POD
- Autoencoders
Reduced Variables
$\mathbf{q}_r$
Learning
Data
- Linear
- Quadratic
- Neural
Non-intrusive Reduced Order Model
$\mathcal{N}(\mathbf{q}_r; \theta) = 0$
$\mathbf{q}_r \in \mathbb{R}^k$

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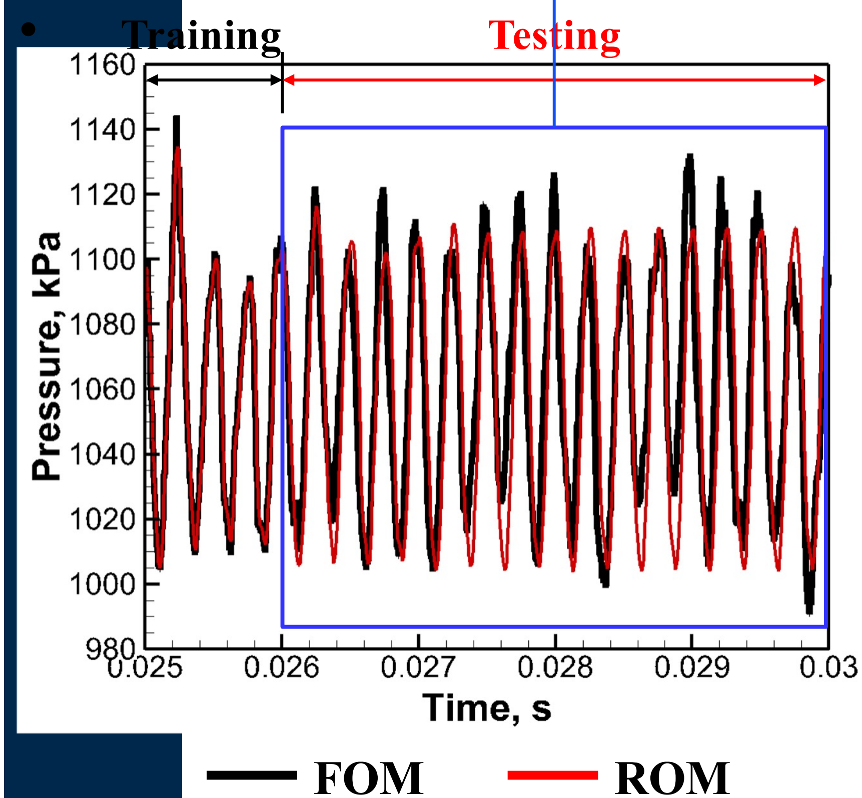
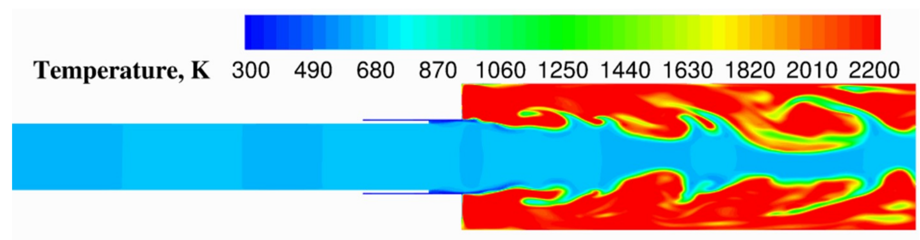
## * Future-state predictions of QoIs

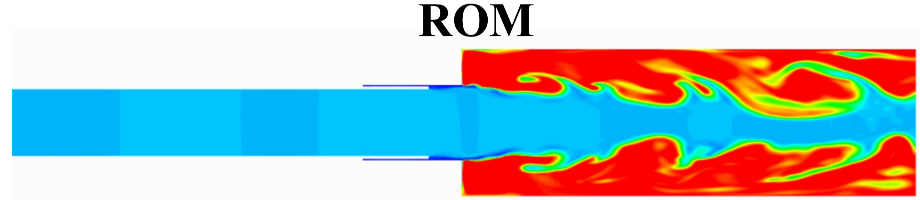



**FOM**




**8h to simulate 1*ms***

**ROM**



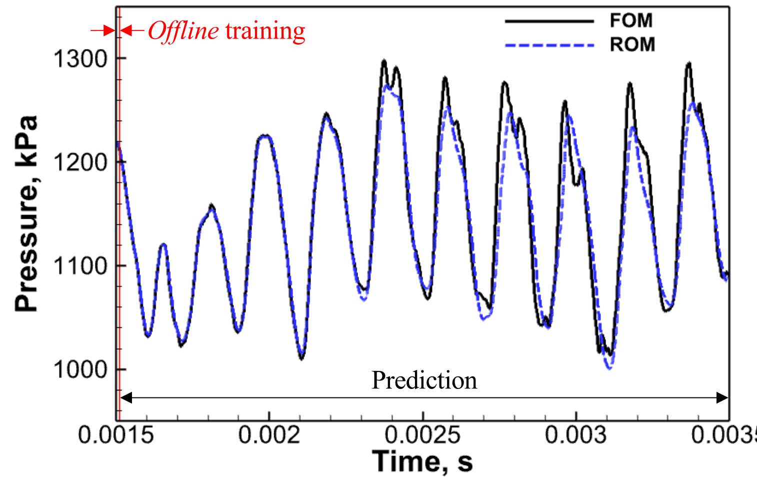
**15 sec to simulate 1*ms* (< 10% error)**

# True predictivity with Adaptive basis & sampling

- Dimension: 5
- Sampling points update  frequency: 20
- Components sampled: 0.5%

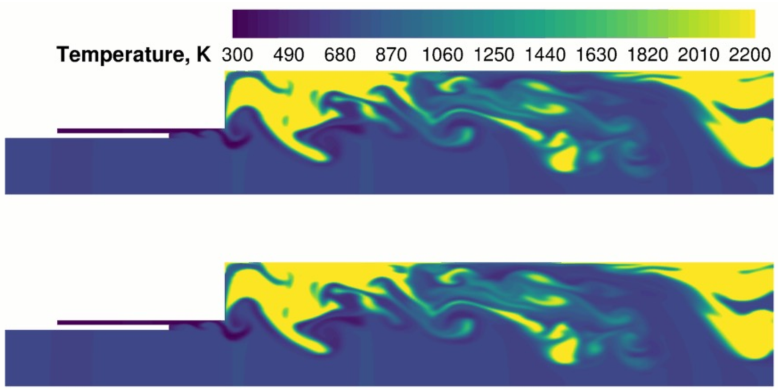
➢0.01*ms offline* training → 2*ms* prediction

***Local*** **Pressure Time Trace**




**FOM**

**ROM**




Sampling Points Adaptation

# Adaptive ROMs enable *transient* & *parametric* predictions

- Dimension: 5
- Sampling points update frequency: 20
- Components sampled: 0.5%

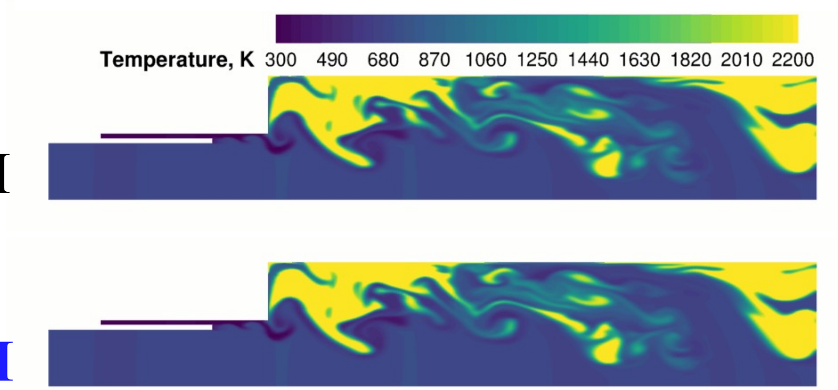
➢ 0.01*ms* *offline* training with 100% $m_{ox}$

→ 2*ms* prediction with $m_{ox}$ reduced to 50%

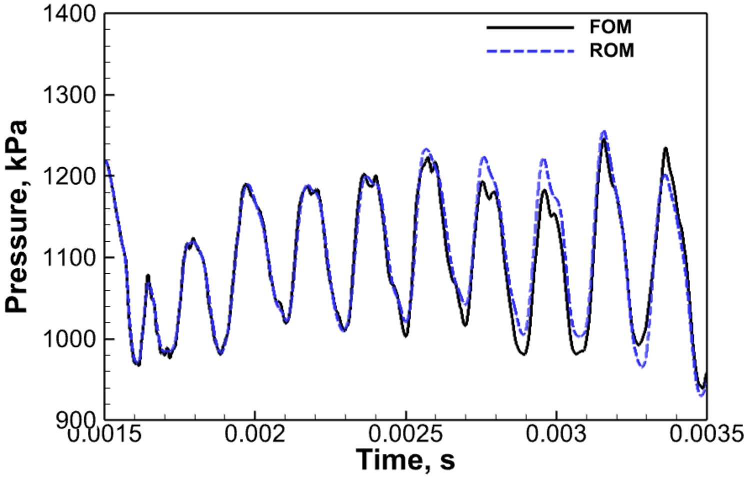
* $m_{ox}$ reduced by 50%

FOM

ROM




***Local* Pressure Time Trace**



# Resources

https://caslab.engin.umich.edu/teaching

- Isaac Newton Institute tutorial on Model Order reduction for complex systems (Jan 2023)
  1. Model Order Reduction theory manual
     http://websites.umich.edu/~caslab/docs/Newton/MOR_Theory.pdf
  2. PERFORM (Prototyping environment for reacting flow order reduction methods : code)
  3. PERFORM (Prototyping environment for reacting flow order reduction methods : doc)
  4. Slides (coming soon)

Also: https://afcoe.engin.umich.edu/publications

# Benchmarking & Broader Engagement

- Workshop to tackle ROMs for a hierarchy of challenging (yet manageable) multi-species/reacting flows
- 2D model combustor dataset publicly available

https://romworkshop.engin.umich.edu/

- Companion code: PERFORM (Prototyping EnviRonment FOr Reduced Modeling)
- Open-source Python 1D reacting flow finite volume solver / ROMs
- Framework designed to easily implement and test new ROM methods on simplified reacting flow problems

https://github.com/cwentland0/perform

USER GUIDE
Quick Start
Example Cases
Inputs
Outputs
Input Parameter Index
Miscellanea
Issues and Contributing

SOLVER
Governing Equations
Flux Schemes
Gradient Limiters
Boundary Conditions
Time Integrators
Gas Models
Reaction Models

ROMS
Reduced-order Modeling
ROM Input Files
∃ Linear Subspace Projection ROMs
Galerkin Projection
LSPG Projection
SP-LSVT Projection
Non-linear Subspace Projection ROMs



# Linear Subspace Projection ROMs

We begin describing linear projection ROMs by defining a general non-linear ODE which governs our dynamical system, given by

$$\frac{d\mathbf{q}}{dt} = \mathbf{R}(\mathbf{q})$$

where for ODEs describing conservation laws, $\mathbf{q} \in \mathbb{R}^N$ is the conservative state, and the non-linear right-hand side (RHS) term $\mathbf{R}(\mathbf{q})$ is the spatial discretization of fluxes, source terms, and body forces. For linear subspace ROMs, we make an approximate representation of the system state via a linear combination of basis vectors,

$$\mathbf{q} \approx \widetilde{\mathbf{q}} = \overline{\mathbf{q}} + \mathbf{P} \sum_{i=1}^{K} \mathbf{v}_i \hat{q}_i = \overline{\mathbf{q}} + \mathbf{P}\mathbf{V}\widehat{\mathbf{q}}$$

The basis $\mathbf{V} \in \mathbb{R}^{N \times K}$ is referred to as the "trial basis", and the vector $\widehat{\mathbf{q}} \in \mathbb{R}^K$ are the generalized coordinates. The matrix $\mathbf{P}$ is simply a constant diagonal matrix which scales the model prediction. $K$, sometimes referred to as the "latent dimension", is chosen such that $K \ll N$. By far the most popular means of computing the trial basis is the proper orthogonal decomposition method.

Inserting this approximation into the FOM ODE, projecting the governing equations via the "test" basis $\mathbf{W} \in \mathbb{R}^{N \times K}$, and rearranging terms arrives at

$$\frac{d\widehat{\mathbf{q}}}{dt} = \left[\mathbf{W}^T\mathbf{V}\right]^{-1} \mathbf{W}^T \mathbf{P}^{-1} \mathbf{R}\left(\widetilde{\mathbf{q}}\right)$$

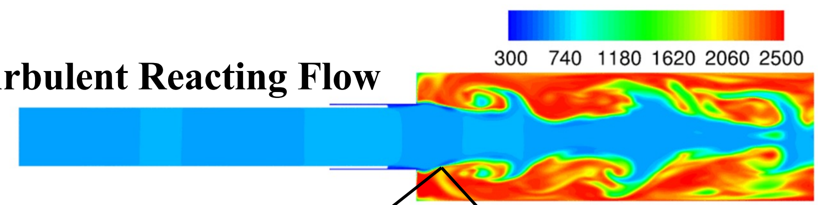
This is now a $K$-dimensional ODE which may be evolved with any desired time integration scheme

# Established test suites for ROM (Release 1.0)

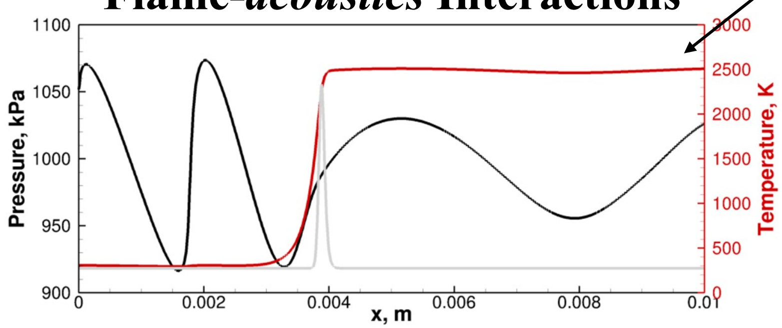
**1D convection-dominated problems with *sharp gradients* and *multi-scale physics***

- Isolated challenges observed in **turbulent flows *with* reaction**
- Challenging but easily accessible problems to attract more participants

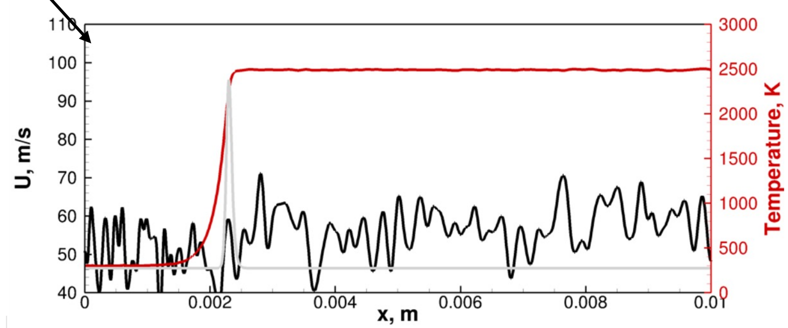
**Turbulent Reacting Flow**




**Flame-*acoustics* Interactions**




**Flame-*turbulence* Interactions**




**https://romworkshop.engin.umich.edu/test-cases**