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

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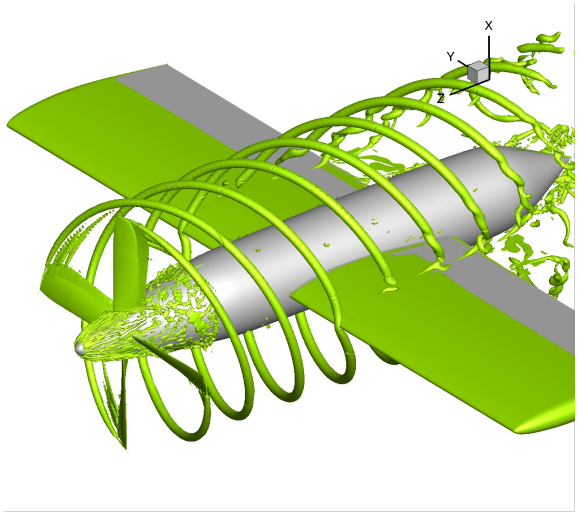
caslab.engin.umich.edu & afcoe.engin.umich.edu

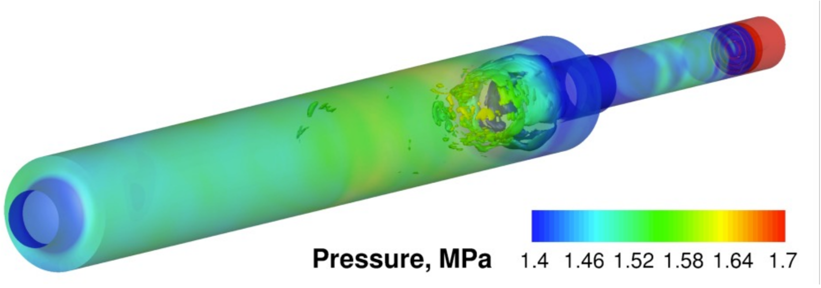
Computational Aerosciences Laboratory

We are a computational modeling group. We build models of real-world problems and we develop theory, algorithms and approaches to enable the construction of such models.

Our work targets applications at a fundamental level (e.g. analyzing basic physical phenomena) all the way to a system-level setting (e.g. models for control)

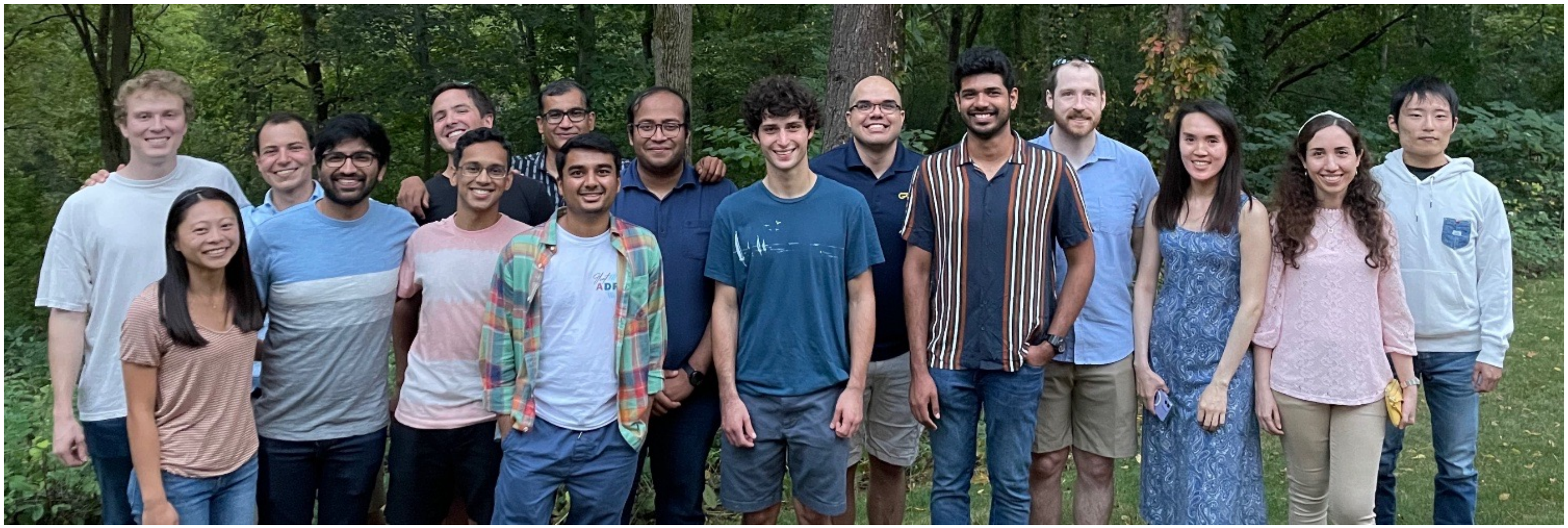
Overarching themes in our lab include complexity reduction, and the development and application of "appropriate'' fidelity models to answer a spectrum of scientific and engineering questions.
Visit us at *caslab.engin.umich.edu*





People

People



Cheng Huang

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+ Center of Excellence Team (afcoe.engin.umich.edu)

Acknowledgment

Outline

- Introduction (today)
- Theory (today)
- Practice (tomorrow)
- The leading edge (tomorrow)

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
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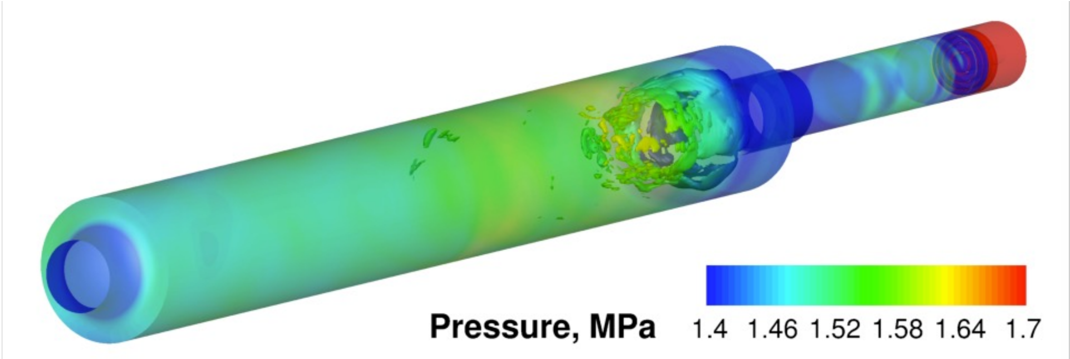
  4. Slides (coming soon)

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

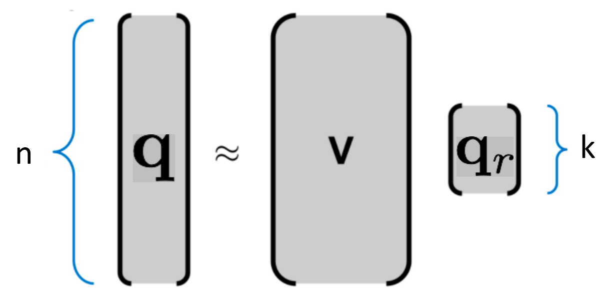
Convection + diffusion + source

$$\frac{\mathrm{d}\mathbf{q}(t,\mathbf{p})}{\mathrm{d}t} = \mathbf{f}(\mathbf{q}(t,\mathbf{p})) \quad ; \quad \mathbf{q} \in \mathbb{R}^n$$ **HFM** $n \sim O(10^9)$

$$\frac{\mathrm{d}\mathbf{q}_r(t,\mathbf{p})}{\mathrm{d}t} = \mathbf{f}_r(\mathbf{q}_r(t,\mathbf{p})) \quad ; \quad \mathbf{q}_r \in \mathbb{R}^k$$ **ROM** $k \sim O(10^3)$

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

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

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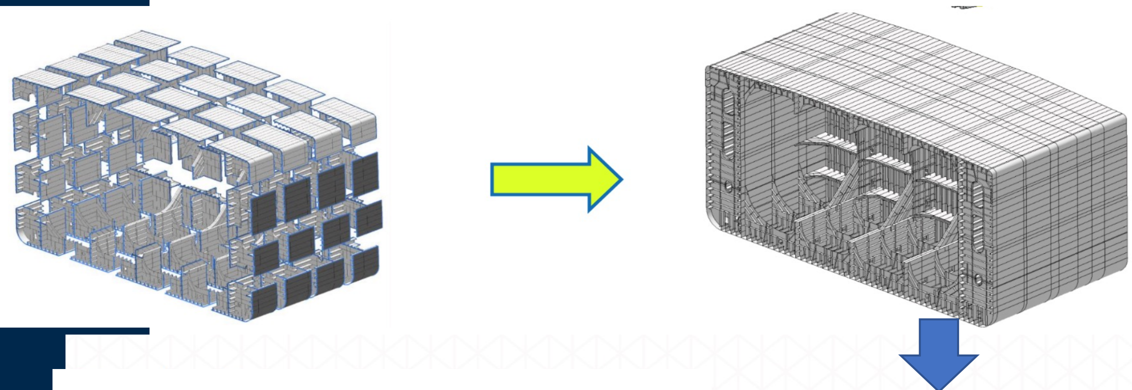

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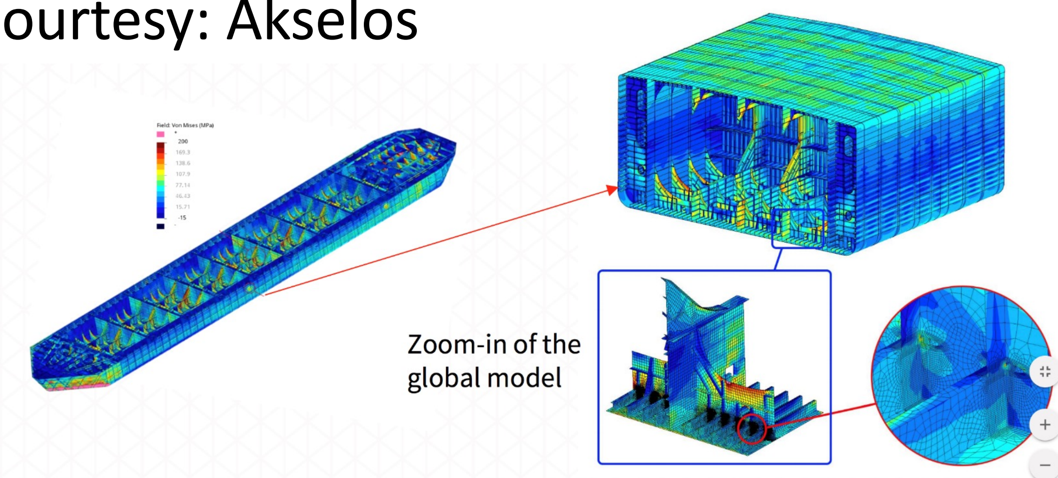

Model Order Reduction

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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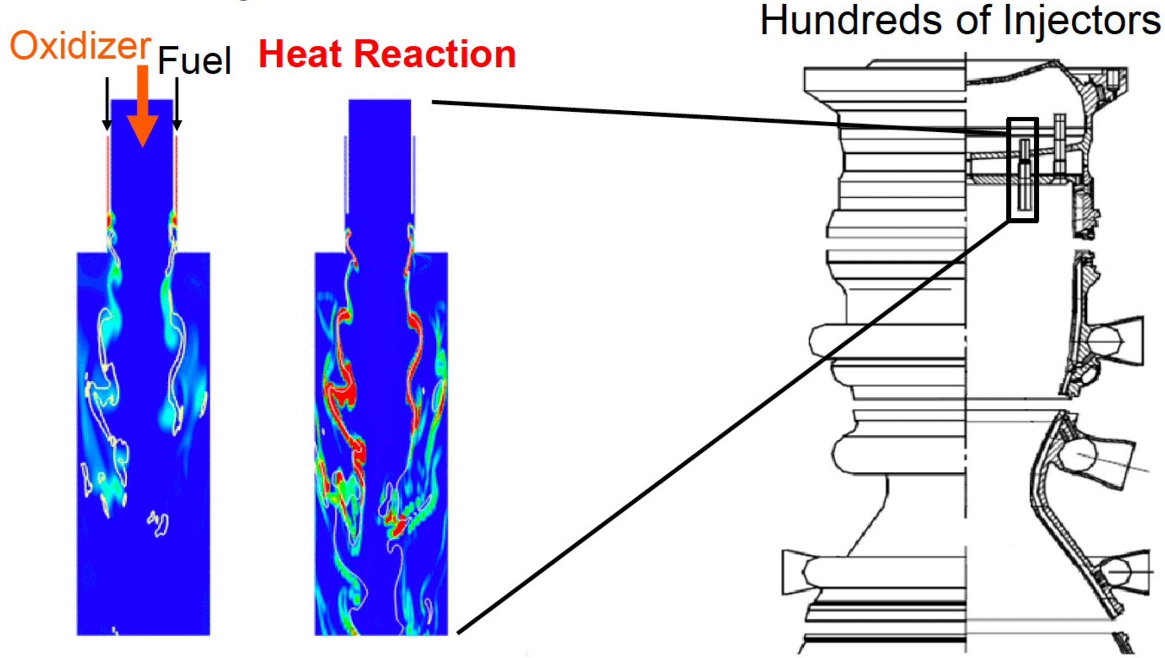
Some Notable advances in ROMs of ‘Complex’ Fluid flows

- 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

FOM of One Injector

Full Scale Engine
Hundreds of Injectors



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

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

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

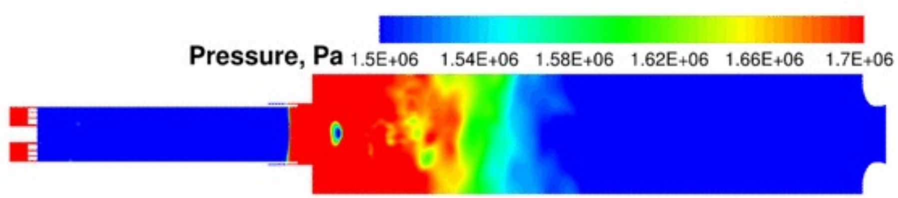
- Non-linear, Multi-scale multi-physics interactions : acoustics, flow & reaction
- Flow – Large coherent structures + small shear layer dynamics
- Reaction – Highly intensive, distributed & intermittent thin flame
- High sensitivity to parameter changes

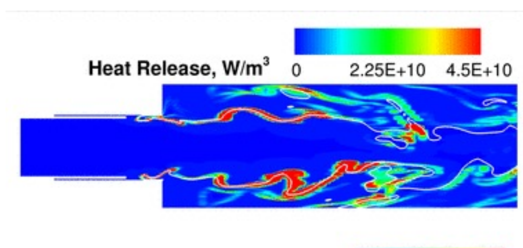
$$\frac{\partial Q}{\partial t} + \frac{\partial F_i}{\partial x_i} + \frac{\partial F_{v,i}}{\partial x_i} = H$$

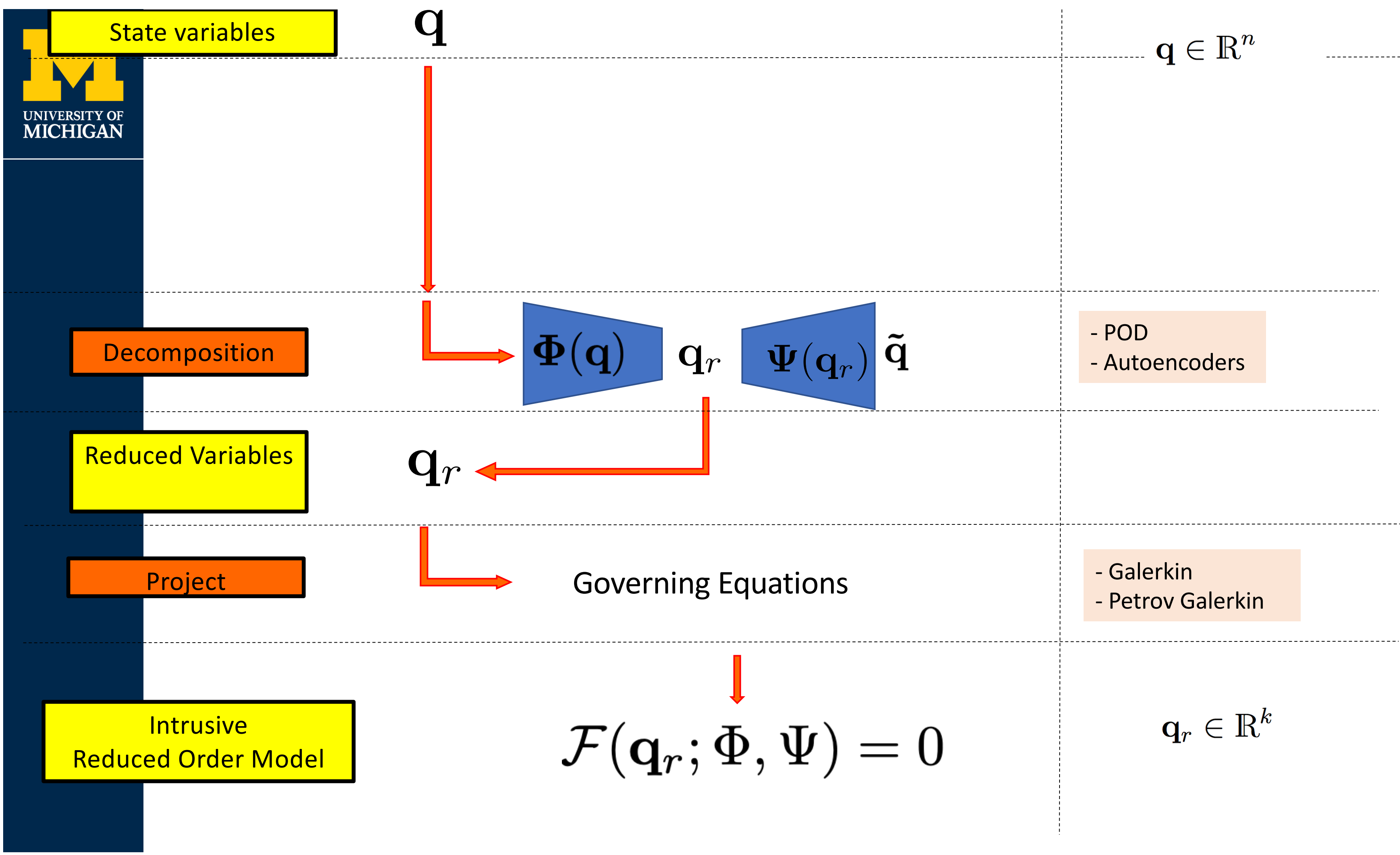
$$Q = \begin{pmatrix} \rho \\ \rho u_i \\ \rho h^0 - p \\ \rho Y_l \end{pmatrix}, \; F_i = \begin{pmatrix} \rho u_i \\ \rho u_i u_j \\ \rho u_i h^0 \\ \rho u_i Y_l \end{pmatrix}, \; F_{v,i} = \begin{pmatrix} 0 \\ \tau_{ij} \\ u_j \tau_{ji} + q_i \\ \rho V_{i,l} Y_l \end{pmatrix}, \; H = \begin{pmatrix}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

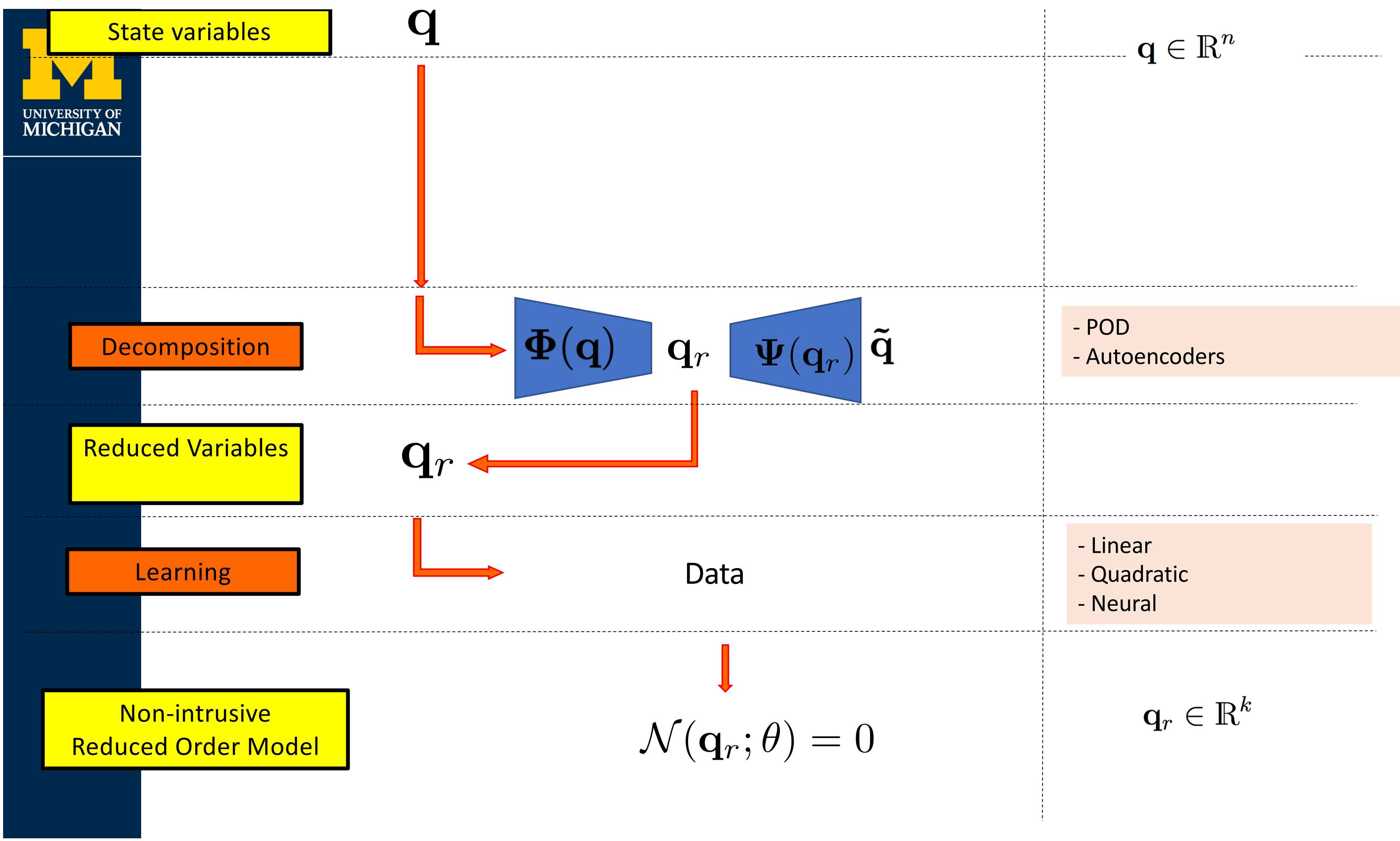
Highly nonlinear and stiff source term :

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



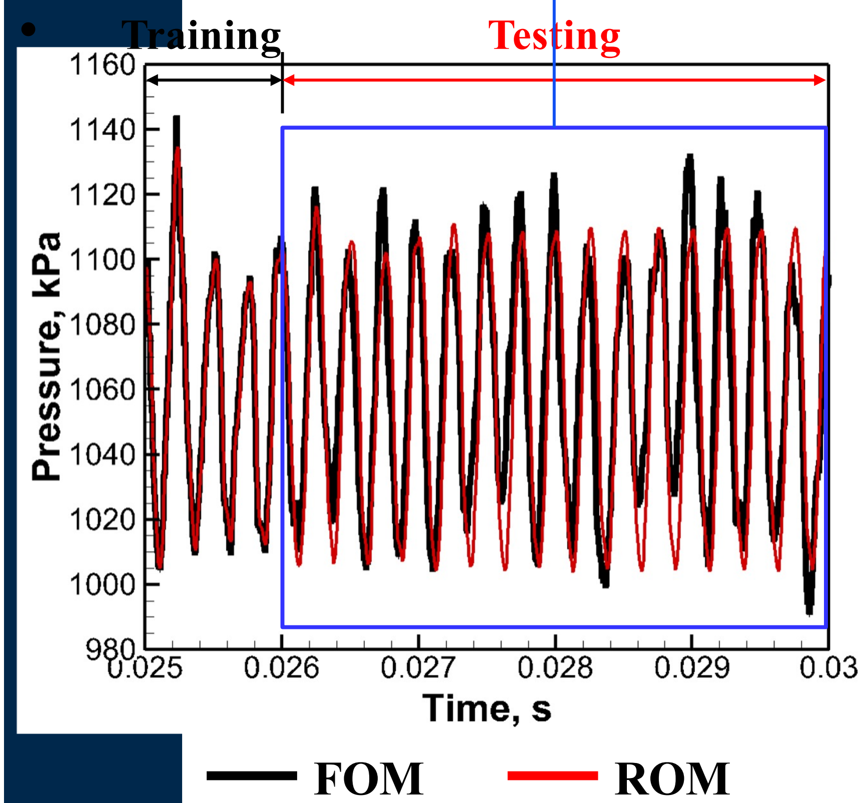



State variables
q
$\mathbf{q} \in \mathbb{R}^n$
Decomposition
$\Phi(\mathbf{q})$
$\mathbf{q}_r$
$\Psi(\mathbf{q}_r)$
$\tilde{\mathbf{q}}$
- POD
- Autoencoders
Reduced Variables
$\mathbf{q}_r$
Project
Governing Equations
- Galerkin
- Petrov Galerkin
Intrusive
Reduced Order Model
$\mathcal{F}(\mathbf{q}_r;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

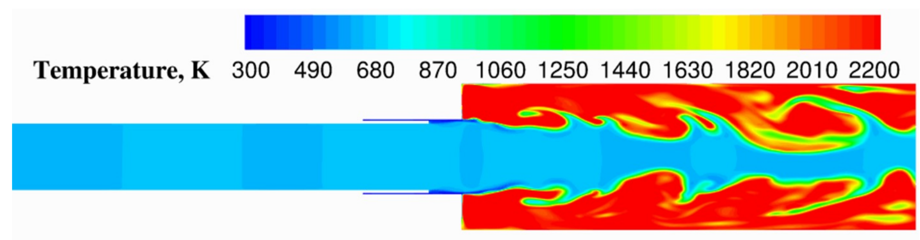


State variables
$\mathbf{q}$
$\mathbf{q} \in \mathbb{R}^n$
Decomposition
$\mathbf{\Phi}(\mathbf{q})$
$\mathbf{q}_r$
$\mathbf{\Psi}(\mathbf{q}_r)$
$\tilde{\mathbf{q}}$
- POD
- Autoencoders
Reduced Variables
$\mathbf{q}_r$
Learning
Data
- Linear
- Quadratic
- Neural
Non-intrusive
Reduced Order Model
$\mathcal{N}(\mathbf{q}_r;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

* Future-state predictions of QoIs

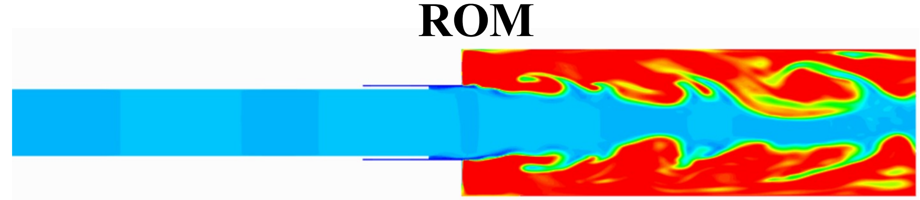


FOM



8h to simulate 1*ms*

ROM

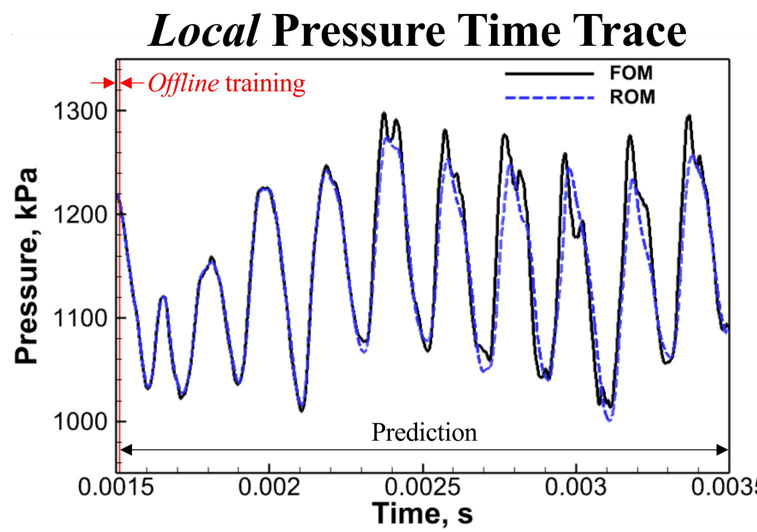


15 sec to simulate 1*ms* (< 10% error)

True predictivity with Adaptive basis & sampling

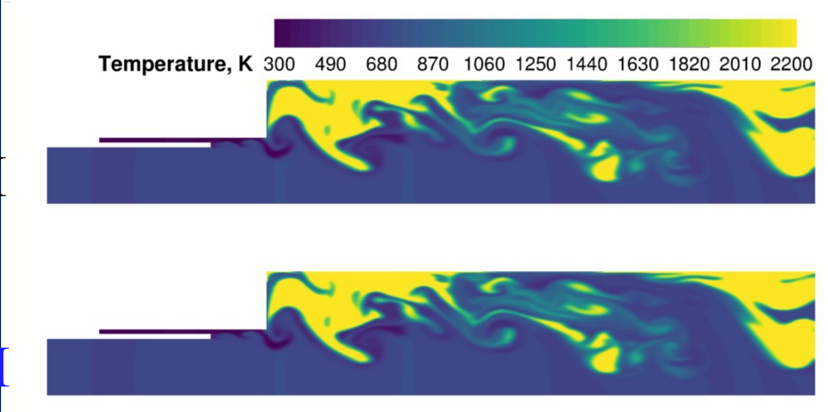
- Dimension: 5
- Sampling points update frequency: 20
- Components sampled: 0.5%

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



FOM

ROM



Sampling Points Adaptation

Adaptive ROMs enable *transient* & *parametric* predictions

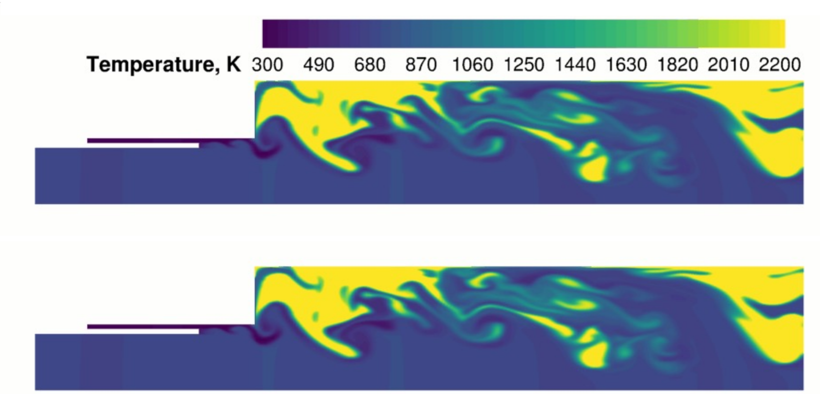
- Dimension: 5
- Sampling points update frequency: 20
- Components sampled: 0.5%

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

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

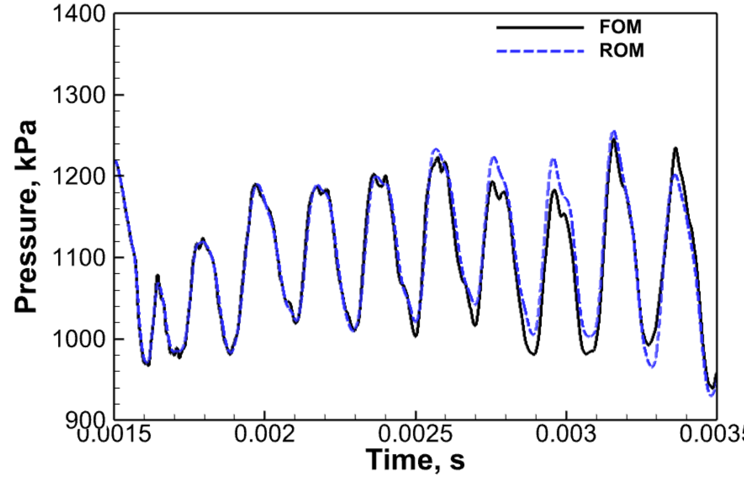
FOM

ROM



* m_{ox} reduced by 50%

***Local* Pressure Time Trace**



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

Model Order Reduction : Theory Guide

Isaac Newton Institute tutorial, Cambridge University

Karthik Duraisamy
Department of Aerospace Engineering
University of Michigan
Ann Arbor, MI 48109

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

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

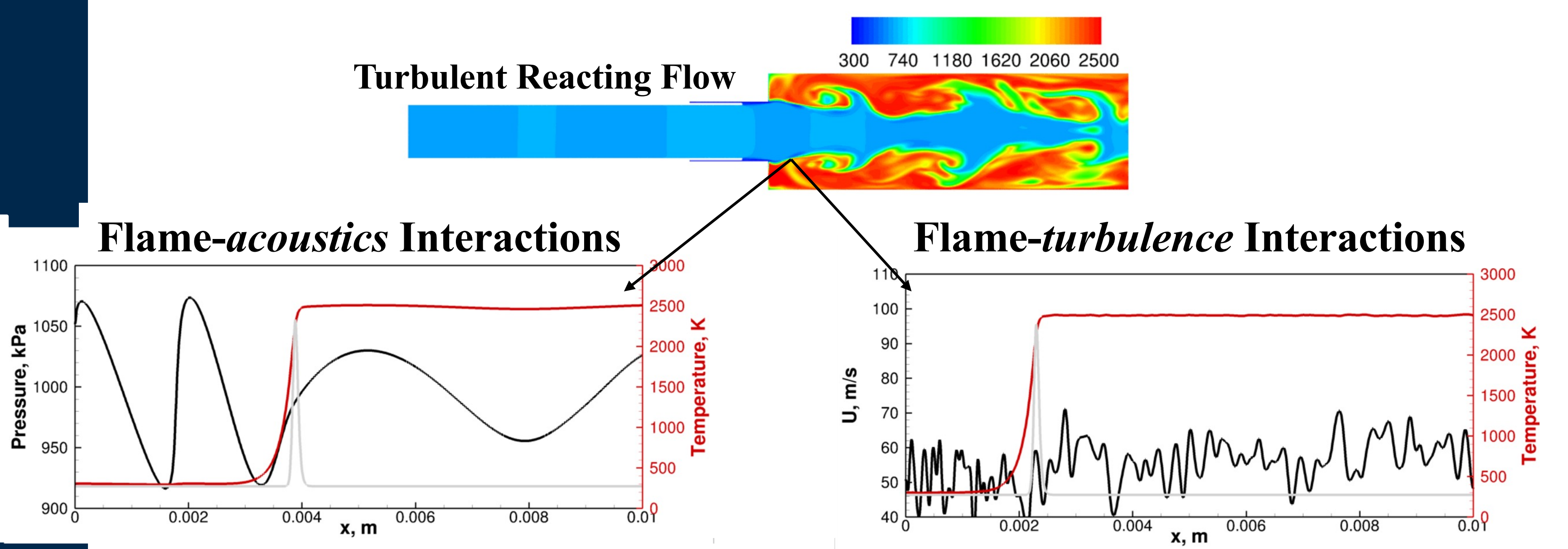
$$\frac{d\widehat{\mathbf{q}}}{dt} = \left[\mathbf{W}^T\mathbf{V}\right]^{-1}\mathbf{W}^T\mathbf{P}^{-1}\mathbf{R}\left(\widetilde{\mathbf{q}}\right)$$

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



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