MOR Test Case for Combustion Applications:

1) Predicting the solution outside the training window

2) Representing long-term temporal dynamics

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ARIA Online Seminar

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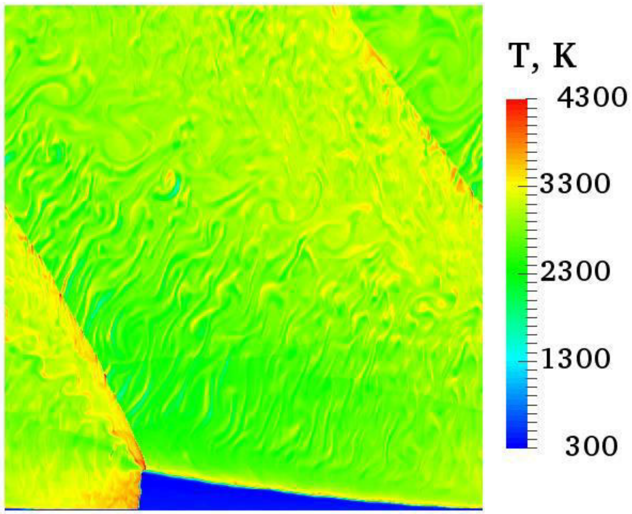
High-fidelity simulations of turbulent combustion are expensive

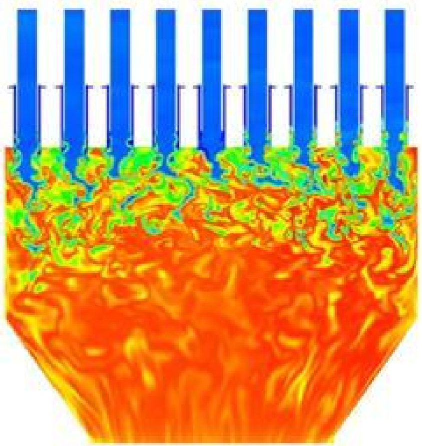
Impractical for practical design !!!

~ 0.1M CPU hours
(per ms)



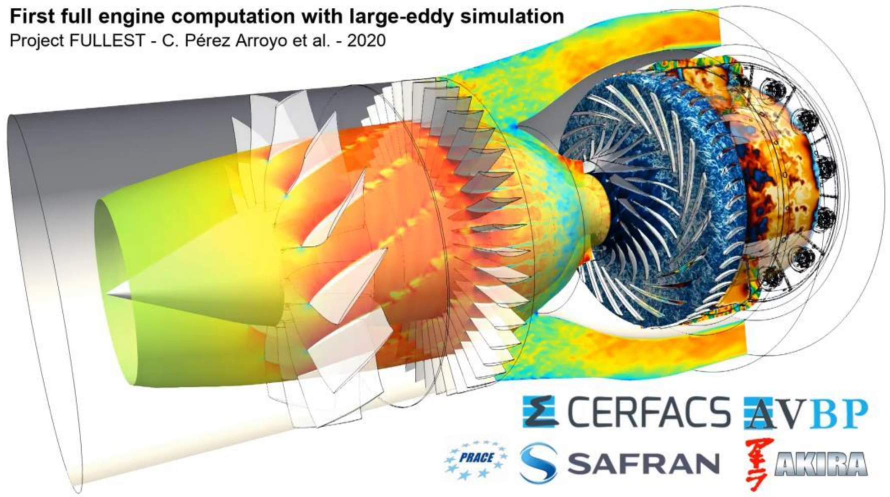
3D RDRE
(Leitz et al., 2019 AIAA SciTech)

~ 0.5M CPU hours
(per ms)



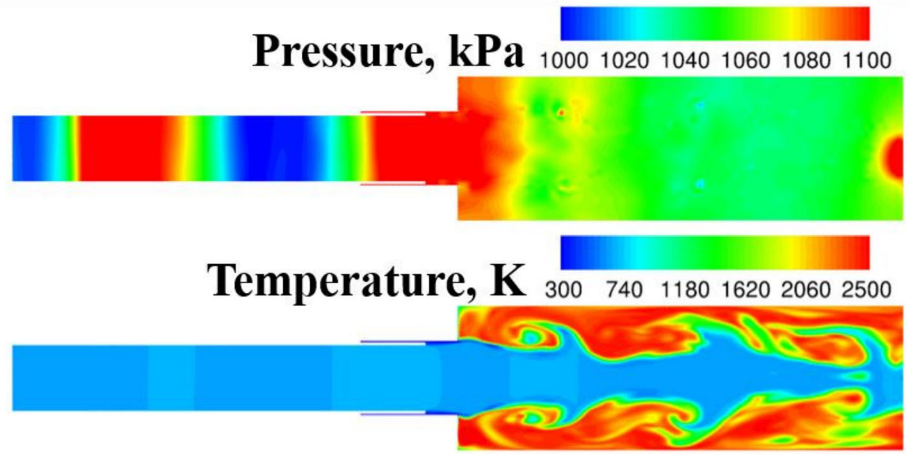
Purdue 9-element transverse chamber
(Harvazinski et al., 2019 AIAA SciTech)

~ 1.7M CPU hours
(per fan turn)

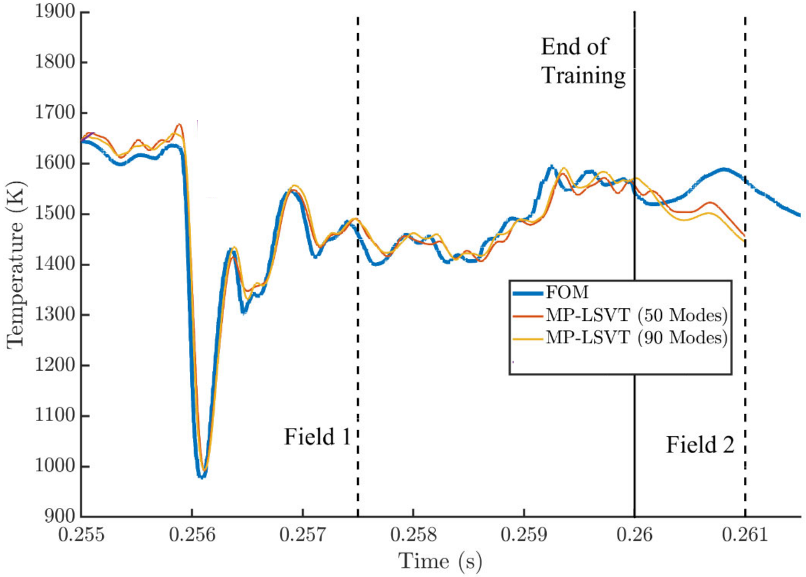


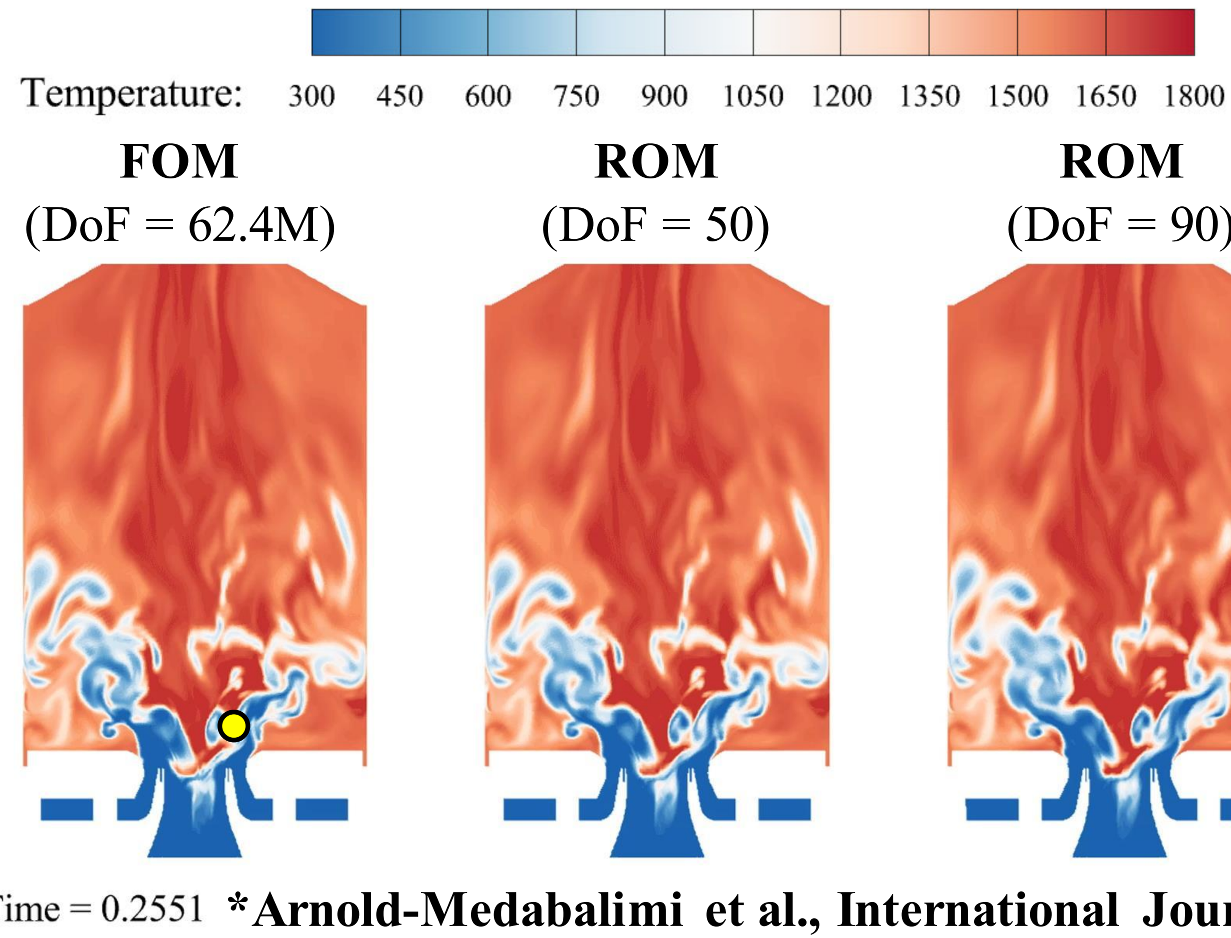
Challenges in MOR Techniques for Combustion Applications

- *Few* applications in **compressible fluid** problems at *scale*
  - Dissimilar multi-scale physics (turbulence, acoustics …)
  - Convection-dominated dynamics
- *Much fewer* activities in **combustion** flows
  - Dispersed steep gradients
  - Highly nonlinear/stiff kinetics
- Prediction beyond training window is challenging
  - Non-stationary chaotic features in flow physics



ROM with linear subspace can *accurately* reproduce but cannot *accurately* predict transport-dominated problems

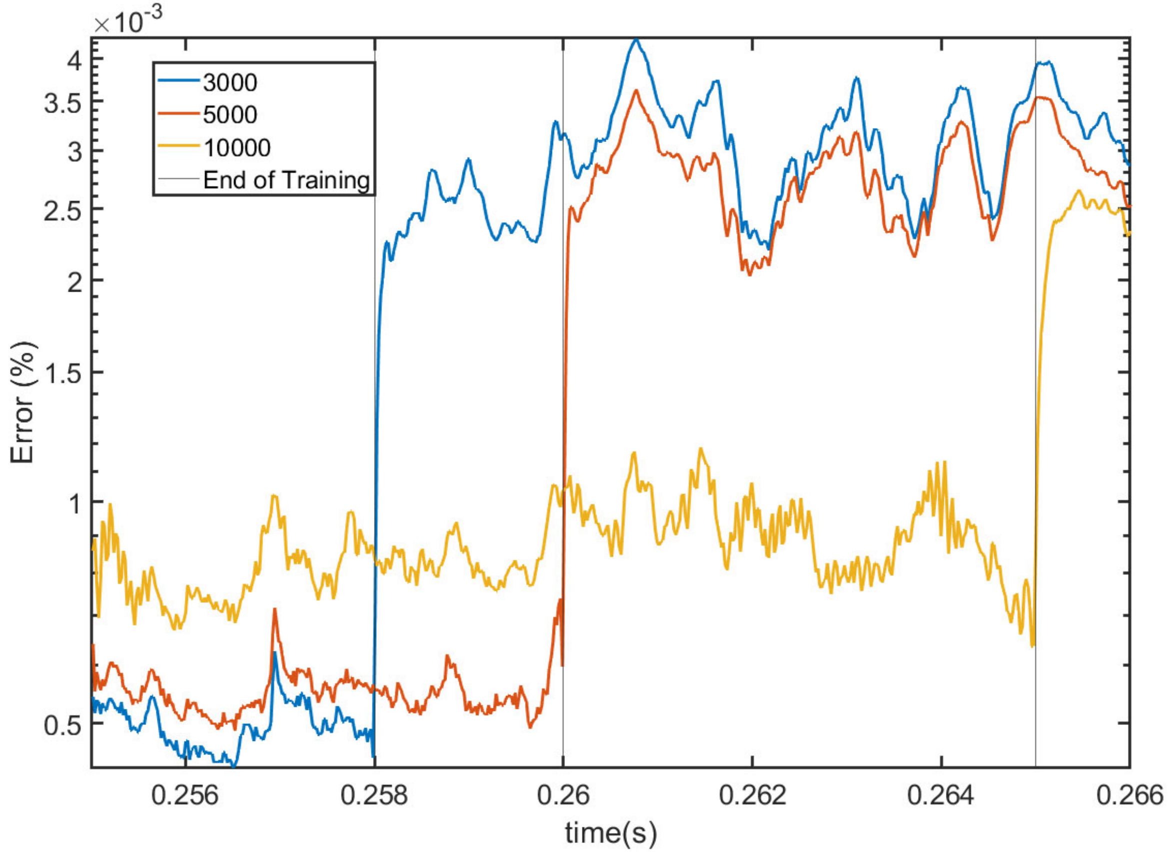




*Arnold-Medabalimi et al., International Journal of Spray and Combustion Dynamics, 2022

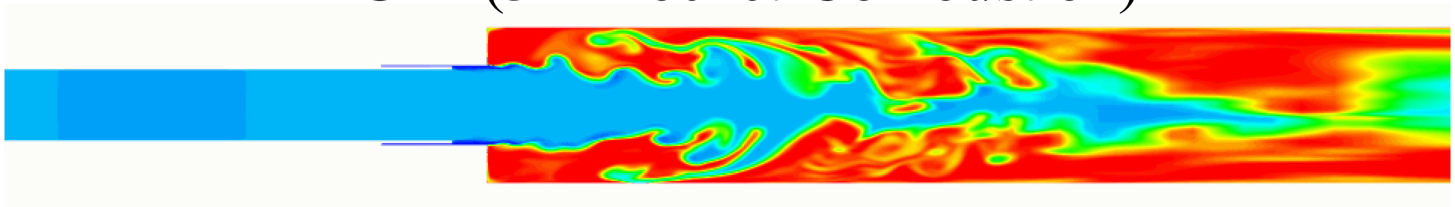
ROM performance is limited by the basis

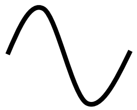
$$\text{Projection Error}(t) = \frac{\left\| \mathbf{q}_{FOM} - \mathbf{V}\mathbf{V}^T \mathbf{q}_{FOM} \right\|_2}{\left\| \mathbf{q}_{FOM} \right\|_2}$$



What is enough training data to predict QoI accurately?

FOM (3D Rocket Combustion)

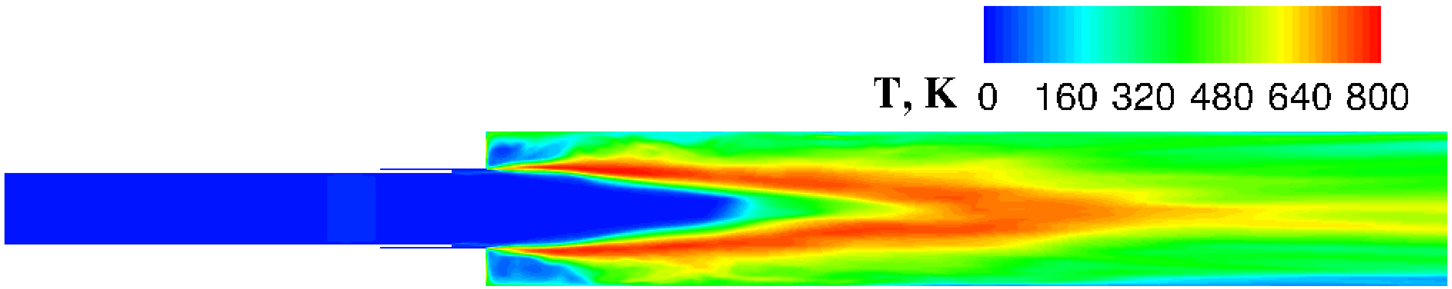




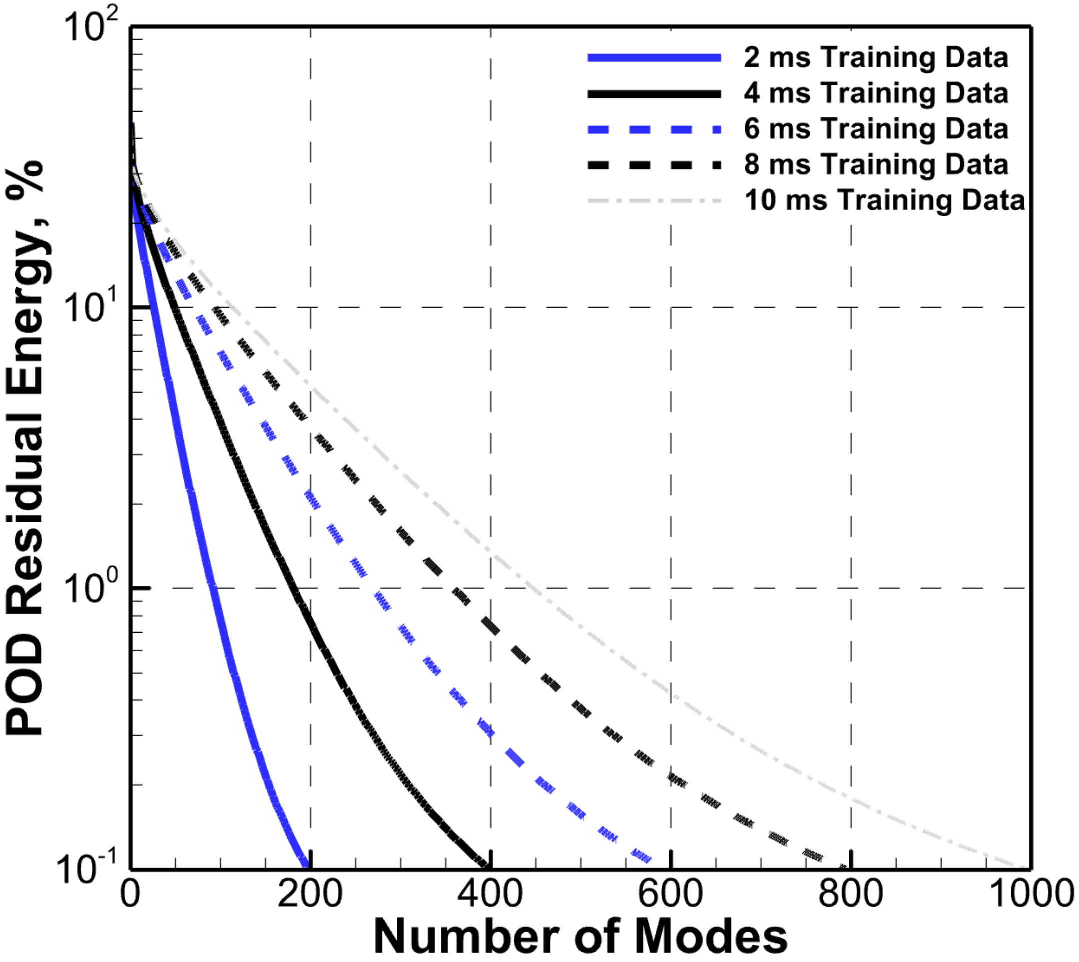
2000Hz @ 10%

QoI – Temperature RMS

calculated based on **10ms** unsteady solutions



POD Energy Decay *vs* Training Data Amount



Slow decays of Kolmogorov N-width with linear subspace approximation

- Significant number of basis modes required to recover accurate representations of the target physics

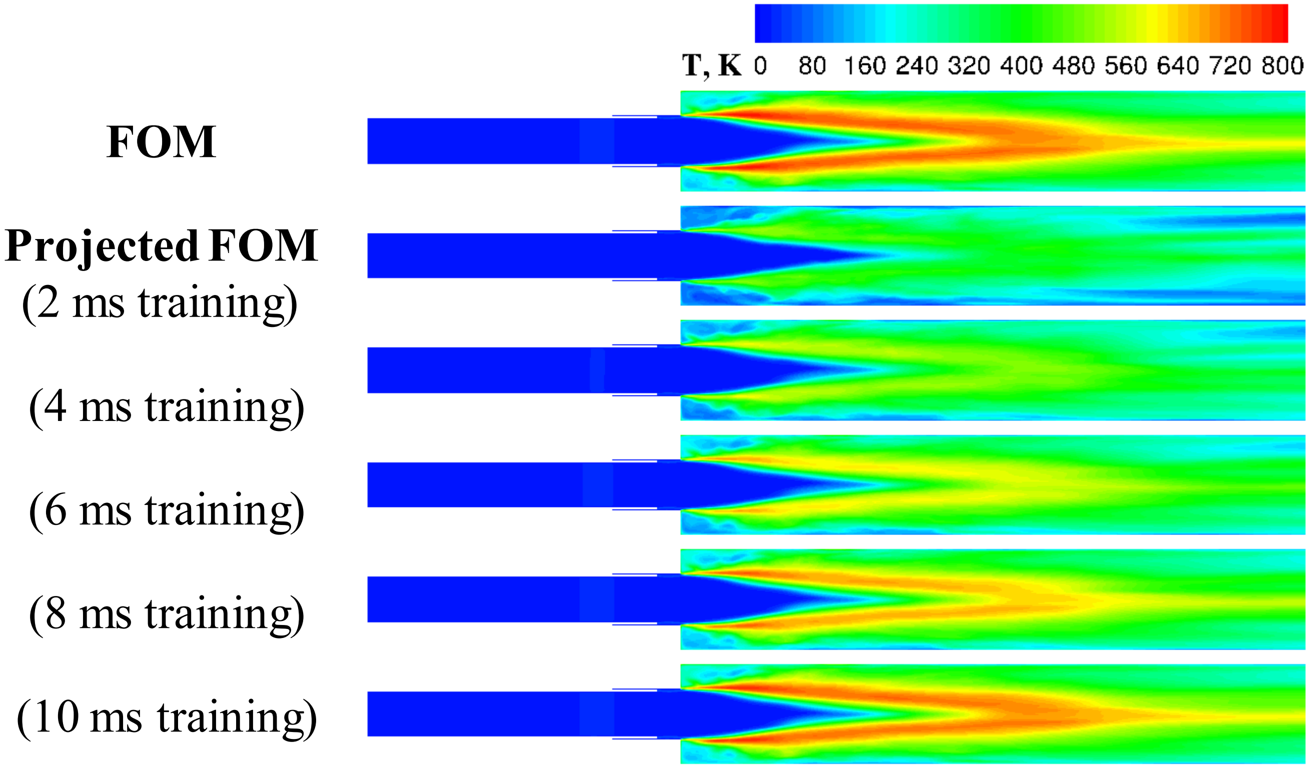
Non-convergence of low-rank approx. versus training data amount

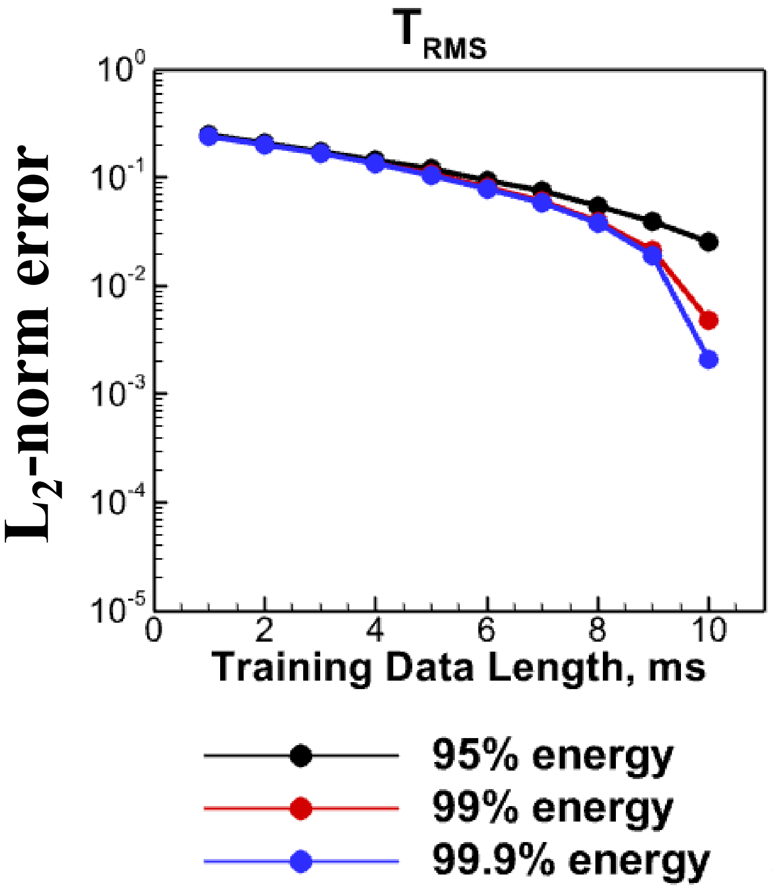
- Predictions of *unseen* physics requires significant amount of training data

Offline Evaluations based on Projected FOM (VV^Tq_{FOM})

- challenging to use *linear static* basis to predict rocket combustion

> 80% training data needed to reach satisfying accuracy in QoI

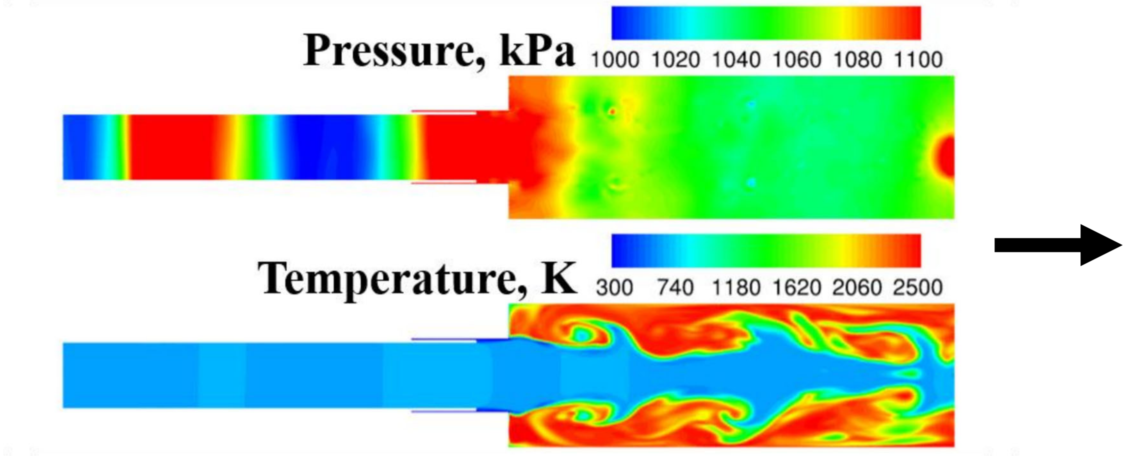


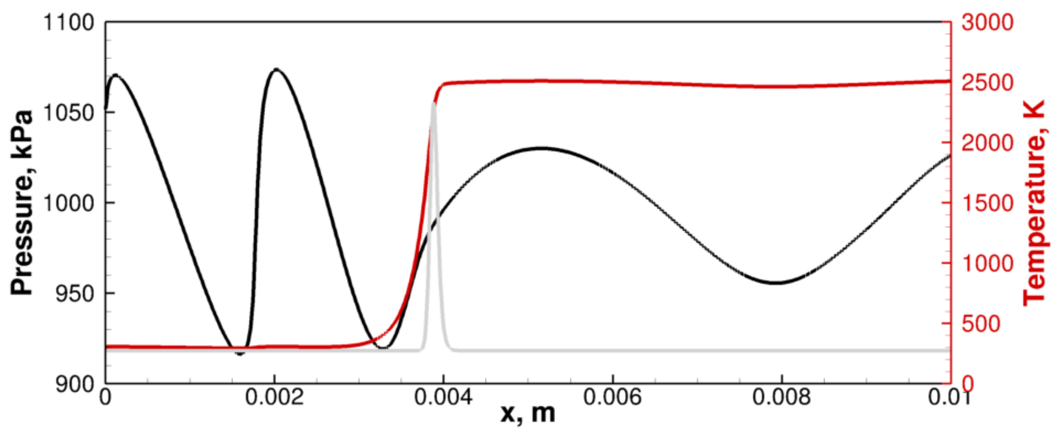


Test Case (Release 1.0)

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

Governing Equation of FOM

$$\frac{\partial Q}{\partial t}+\frac{\partial E}{\partial x}-\frac{\partial E_v}{\partial x}=H$$

where $$Q=\begin{pmatrix}\rho\\ \rho u\\ \rho h^0-p\\ \rho Y_k\end{pmatrix},\ E=\begin{pmatrix}\rho u\\ \rho u^2+p\\ \rho u h^0\\ \rho u Y_k\end{pmatrix},\ E_v=\begin{pmatrix}0\\ \dfrac{4}{3}\mu\dfrac{\partial u}{\partial x}\\ \lambda\dfrac{\partial T}{\partial x}+\displaystyle\sum_{i=1}^{2}\rho D h_i\dfrac{\partial Y_i}{\partial x}\\ \rho D\dfrac{\partial Y_k}{\partial x}\end{pmatrix},$$ and $$H=\begin{pmatrix}0\\ 0\\ 0\\ \dot{\omega}_k\left(Y_k,T,\rho\right)\end{pmatrix}$$

and $\rho=\left(\displaystyle\sum_{k=1}^{N_s}\frac{Y_k}{\rho_k}\right)^{-1}$ with $\rho_k=\dfrac{pW_k}{RT}$, $h^0=h+\dfrac{1}{2}u^2=\displaystyle\sum_{k=1}^{N_s}h_kY_k+\frac{1}{2}u^2$ with $h_k=h_k\left(T\right)$

$\lambda=\dfrac{\mu c_p}{\mathrm{Pr}}$ with $\mathrm{Pr}=0.713$ and $D=\dfrac{\mu}{\rho Sc}$ with $Sc=0.62$

https://perform.readthedocs.io/en/latest/solver/goveqs.html

Combustion: a Single-Step Reaction Model

Reaction	A [$1/s \cdot (kmol/m^3)^{(1-a1-a2)} \cdot 1/K^b$]	b	$-E_a/R$ [K]	Order of the reactants
Reactant → Product	2.12×10^{10}	0.0	-24358	$a_1 = 1.0$ and $a_2 = 0.0$

$$\dot{\omega}_l = MW_l \cdot n_l \cdot k_{ov}$$

$$\text{where } k_{ov} = AT^b \exp\left(\frac{-E_a / R}{T}\right)[\mathrm{R}]^{a_1}[\mathrm{P}]^{a_2},\ [\mathrm{R}] = \frac{\rho Y_1}{MW_1} \text{ and } [\mathrm{P}] = \frac{\rho Y_2}{MW_2}$$

l	**1**	**2**
Species	Reactant	Product
MW_l	21.32	21.32
n_l	-1	1

https://perform.readthedocs.io/en/latest/solver/goveqs.html

JOSS
The Journal of Open Source Software

PERFORM: A Python package for developing reduced-order models for reacting fluid flows

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DOI: 10.21105/joss.03428

Software

- Review
- Repository
- Archive

Editor: Kyle Niemeyer
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Summary

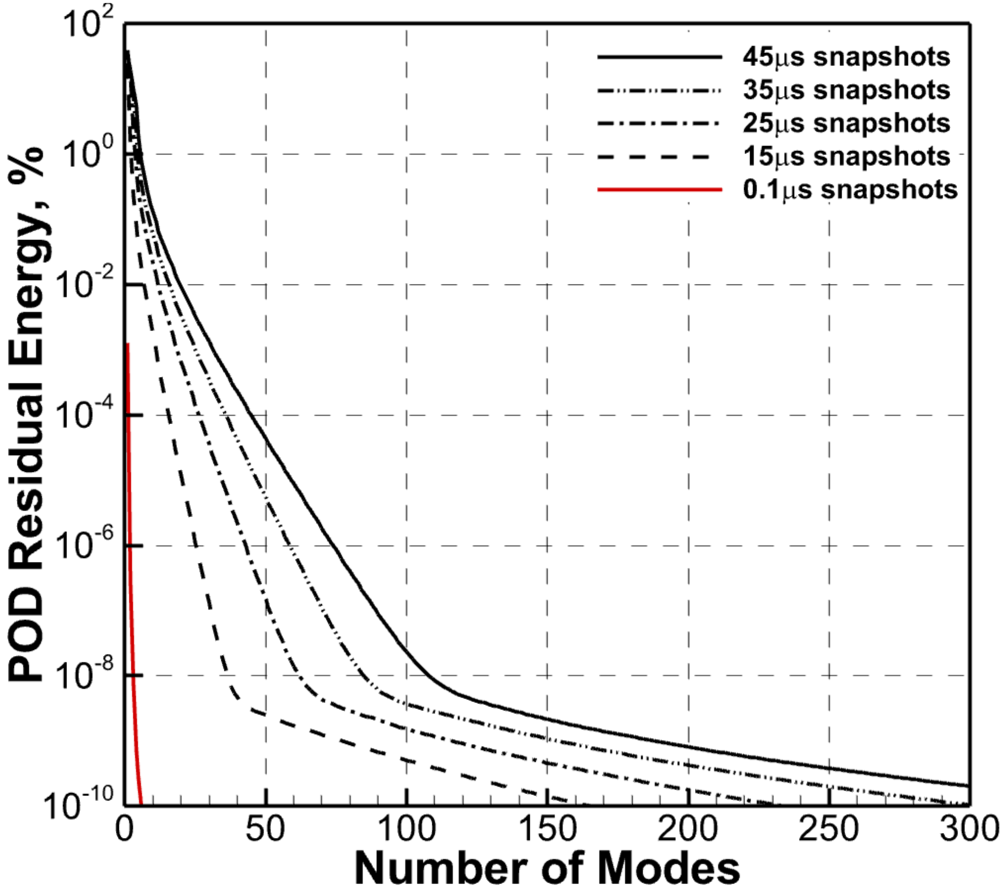
Combusting fluid flows are common in a variety of engineering systems, driving the gas turbines that generate our electricity, providing the thrust for rocket engines, and powering our cars and airplanes. However, the use of computational fluid dynamics (CFD) to simulate these phenomena is practically impossible for time-critical, many-query applications such as parametric design, failure prediction, and uncertainty quantification. Data-driven reduced-order models (ROMs) have shown potential for vastly reducing the computational cost of evaluating CFD models. In general, ROMs learn a low-dimensional representation of the high-dimensional system state (which may be as many as tens or hundreds of millions of degrees of freedom) and evolve this low-dimensional state in time at a much lower computational cost. Research on applying ROMs to practical reacting flows is currently in its early stages, and initial results have shown that standard ROM techniques may be ineffective for this class of problems (Huang et al., 2018; Huang & Duraisamy, 2019). The dearth of research on this topic may be attributed to the complexity of reacting flow modeling combined with a lack of approachable open-source libraries for combustion CFD.

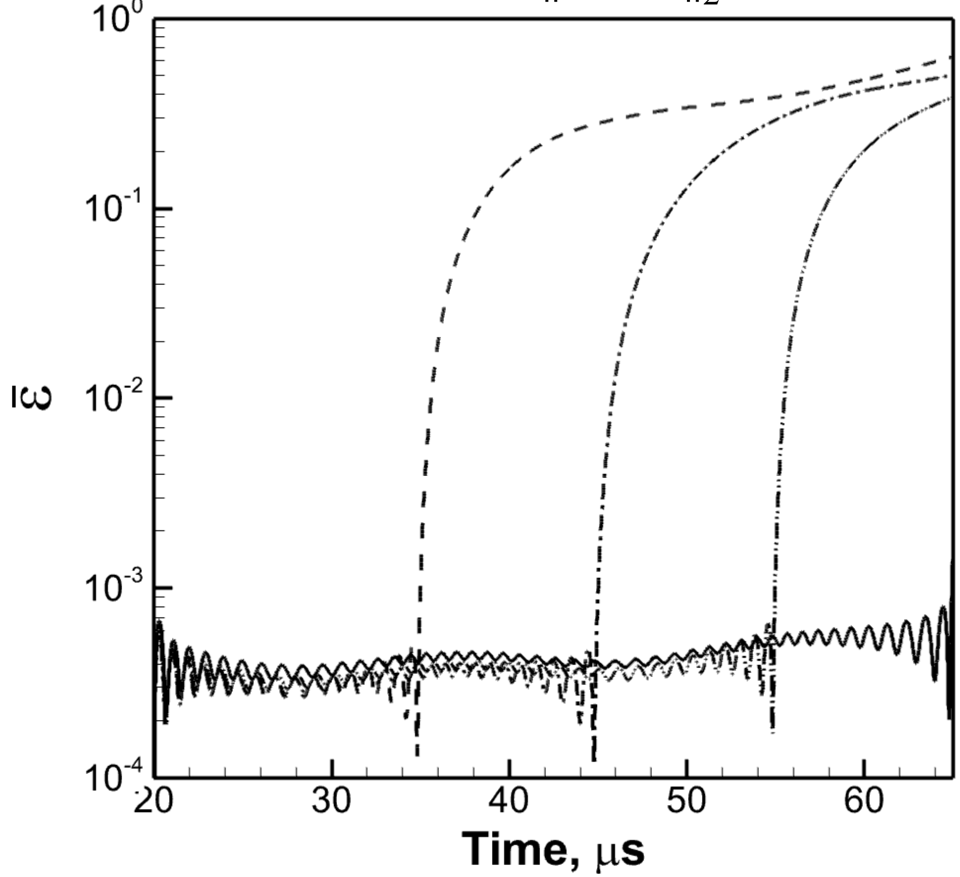
The Prototyping Environment for Reacting Flow Order Reduction Methods (PERFORM) is a Python packaged designed to allow rapid implementation, testing, and evaluation of ROMs for one-dimensional reacting flows. It combines a robust compressible reacting flow solver with a modular framework for deploying new ROM methods. This eliminates much of the software development difficulty for ROM researchers who may have little experience with

https://github.com/cwentland0/perform

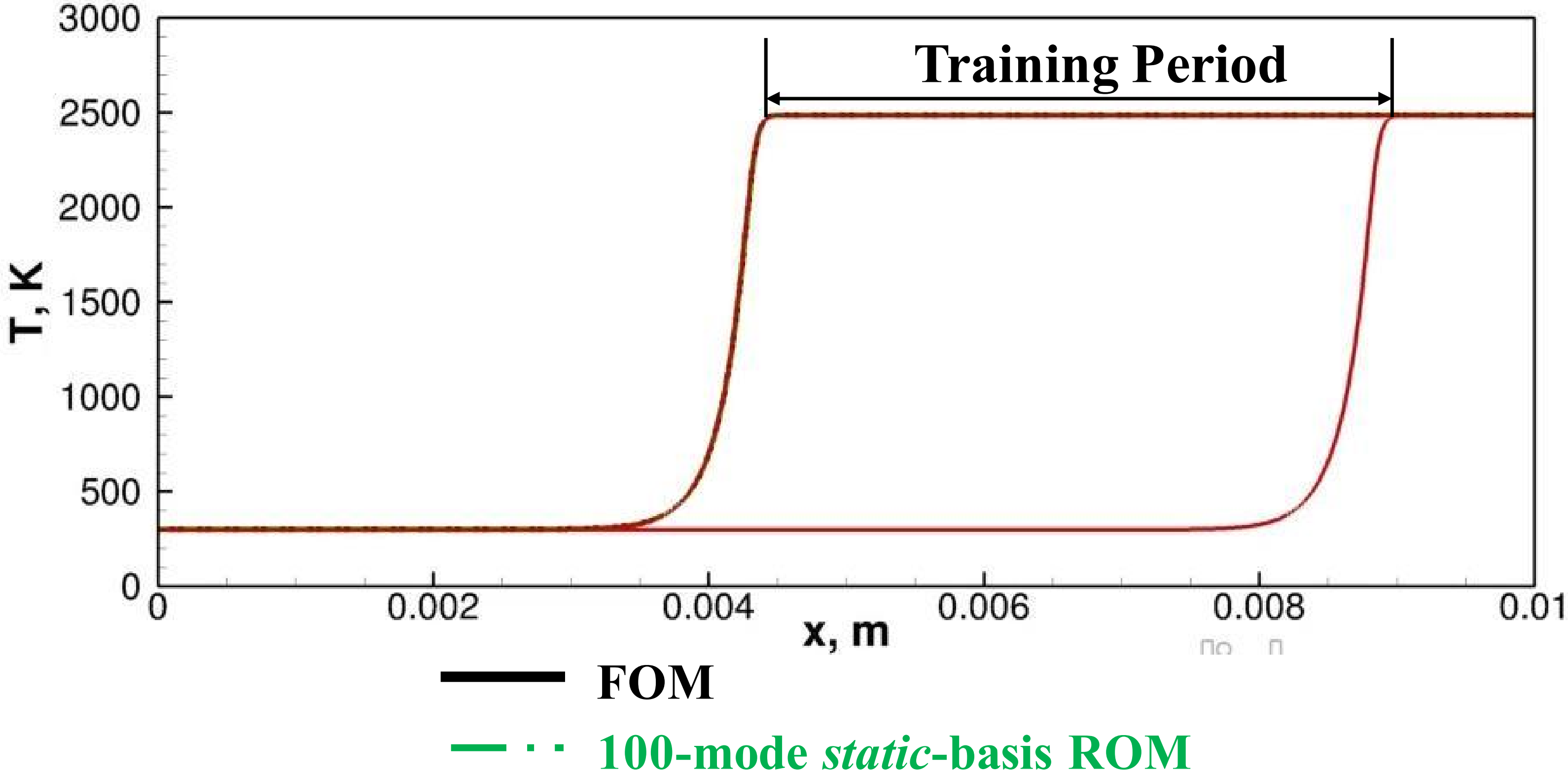
Similar challenges in 1D as the 3D problem

$$\bar{\varepsilon} = \sum_{n=1}^{N_t} \frac{\left\| \mathbf{q}_{FOM}^{n} - \mathbf{V}\mathbf{V}^{T}\mathbf{q}_{FOM}^{n} \right\|_2}{\left\| \mathbf{q}_{FOM}^{n} \right\|_2}$$



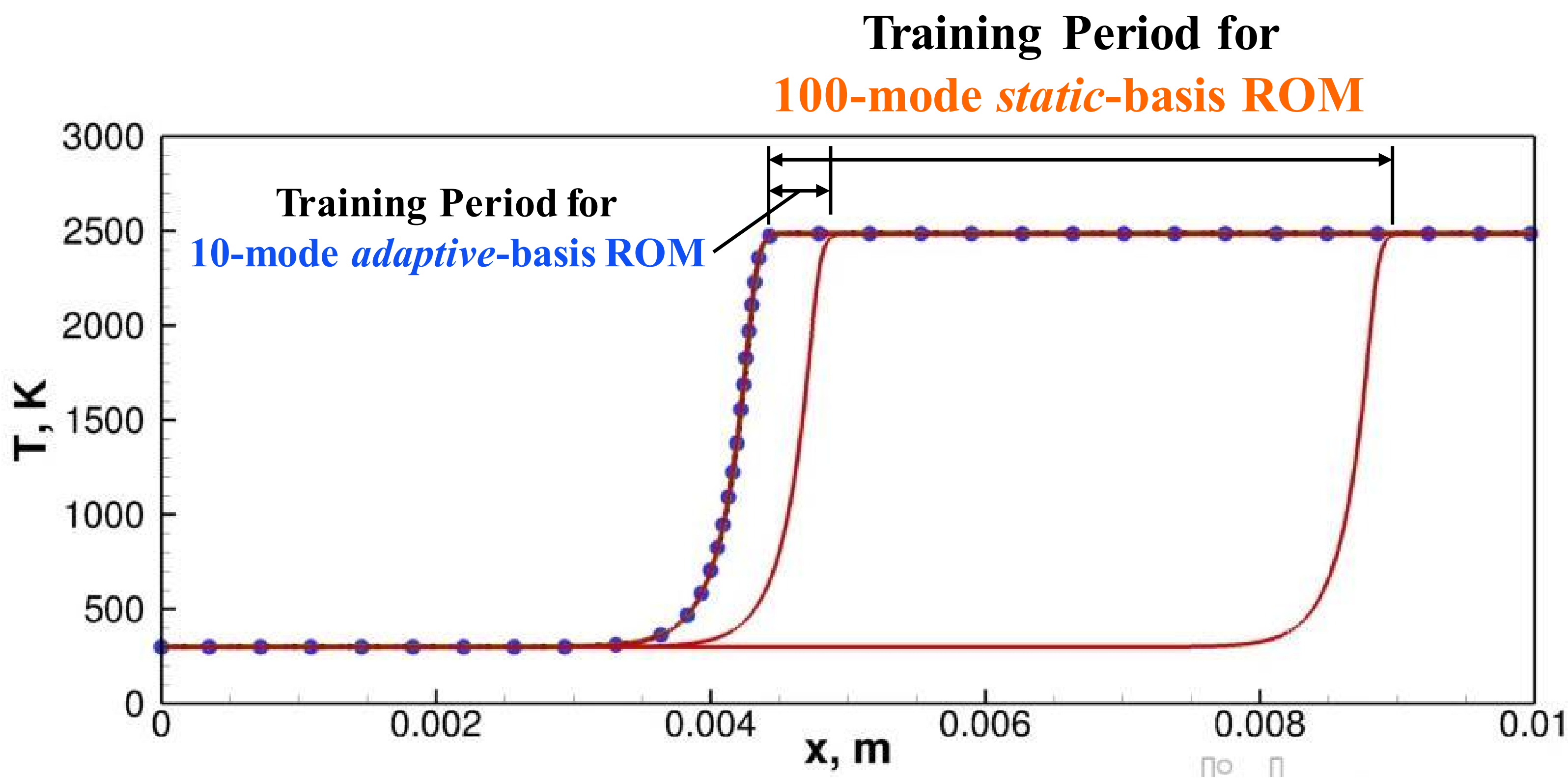


Similar challenges in 1D as the 3D problem



Methods Developed based on the Test Case

- Wentland, C., Huang, C., and Duraisamy, K., "Closure of Reacting Flow Reduced-Order Models via the Adjoint Petrov-Galerkin Method", AIAA Aviation, 2019.
- Uy, W., Wentland, C., Huang, C., and Peherstorfer, B., "Reduced models with nonlinear approximations of latent dynamics for model premixed flame problems", arXiv:2209.06957, 2022.
- Rezaian, E., Huang, C., and Duraisamy, K., "Non-intrusive balancing transformation of highly stiff systems with lightly damped impulse response", Philosophical Transactions of the Royal Society A, 2022.
- Rezaian, E. and Duraisamy, K., "Predictive Modeling of Complex Flows using Regularized Conditionally Parameterized Graph Neural Networks", AIAA SciTech, 2023.
- Huang, C., and Duraisamy, K., "Predictive Reduced Order Modeling of Chaotic Multi-scale Problems Using Adaptively Sampled Projections", arXiv:2301.09006v1, 2023



FOM

100-mode *static*-basis ROM $\tilde{\mathbf{q}}_p = \mathbf{V}\mathbf{q}_r$

10-mode *adaptive*-basis ROM

Peherstorfer, SIAM JSC, 2020

$$\tilde{\mathbf{q}}_p = \mathbf{V}^n\mathbf{q}_r \text{ where } \mathbf{V}^{n+1} = \mathbf{V}^n + \delta\mathbf{V}_n, \ \underset{\delta\mathbf{V}^n}{\arg\min}\left\|\mathbf{V}^{n+1}\left[\left(\mathbf{V}^n\right)^+\mathbf{F}\right] - \mathbf{F}\right\|_F^2$$

Adaptive (basis & sampling) ROM

Huang and Duraisamy, https://arxiv.org/abs/2301.09006

inspired by Peherstorfer, SIAM JSC, 2020

Step 1: Solve *hyper-reduced* ROM to propagate in time

$$\left(\bar{\mathbf{W}}^{n+1}\right)^T \mathbf{V}^n \left(S^n \mathbf{V}^n\right)^+ S^n \mathbf{r}\left(\hat{\mathbf{q}}_r^{n+1}\right) = 0 \;\Rightarrow\; \boxed{\hat{\mathbf{q}}_r^n \rightarrow \hat{\mathbf{q}}_r^{n+1}}$$

Step 2: Evaluate full-state $\hat{\mathbf{q}}_p^{n+1}$ based on full-model equation residual

$$S_n \mathbf{r}\left(\hat{\mathbf{q}}_p^{n+1}\right) = 0 \quad \text{and} \quad \left(I - S_n\right)\mathbf{r}^*\left(\hat{\mathbf{q}}_p^{n+1}\right) = 0$$

Step 3: Update the basis (every z_b time steps)

$$\mathbf{V}^{n+1} = \mathbf{V}^n + \delta\mathbf{V}^n \quad s.t. \quad \underset{\delta\hat{\mathbf{V}}_n}{\arg\min} \left\| \mathbf{V}^{n+1}\left[\left(\mathbf{V}^n\right)^+ \hat{\mathbf{q}}_p^{n+1}\right] - \hat{\mathbf{q}}_p^{n+1} \right\|_2^2$$

Step 4: Update sampling points (every z_s time steps) $\quad S_n \rightarrow S_{n+1}$

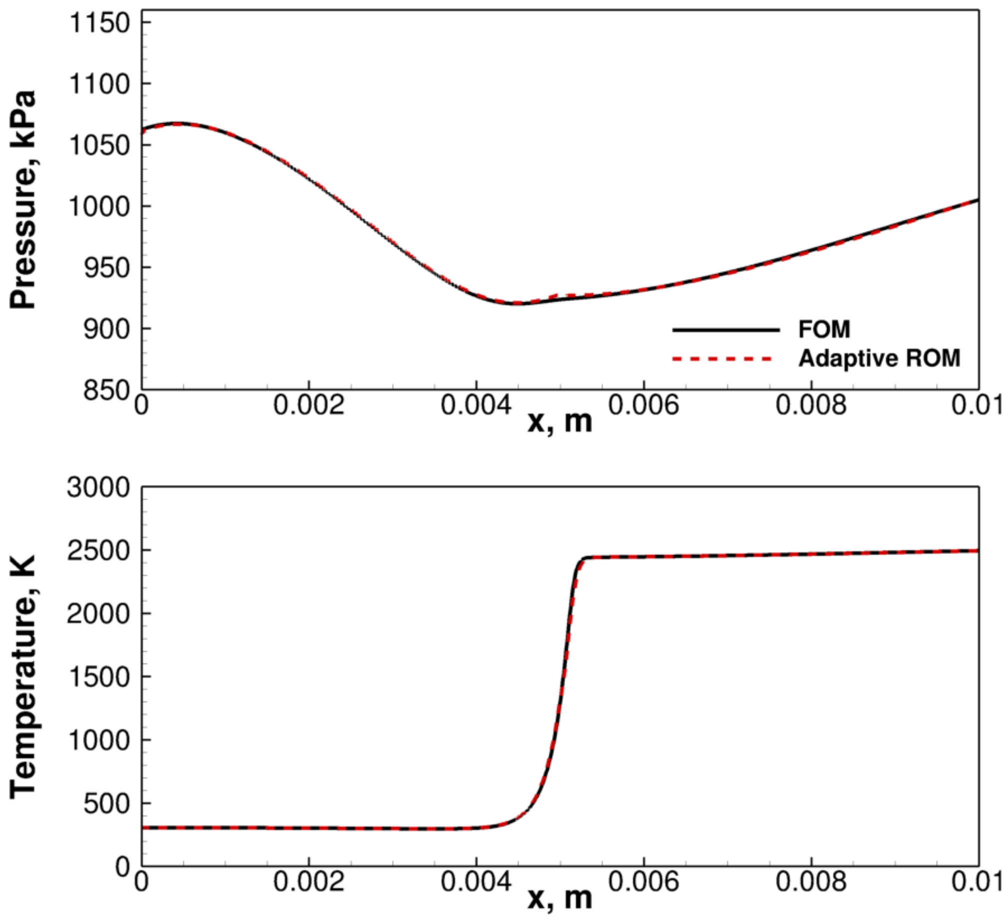
Adaptive ROM: 1D Laminar Flame

Huang and Duraisamy, https://arxiv.org/abs/2301.09006

- *offline* training: 10 snapshots
- online testing: 4500 snapshots
- Dimension: 5 + Sampling points update time steps (z_s): 50 + Points sampled: 1.0%

→ ~ **O(20) acceleration**

*** Test cases available at**
https://romworkshop.engin.umich.edu/

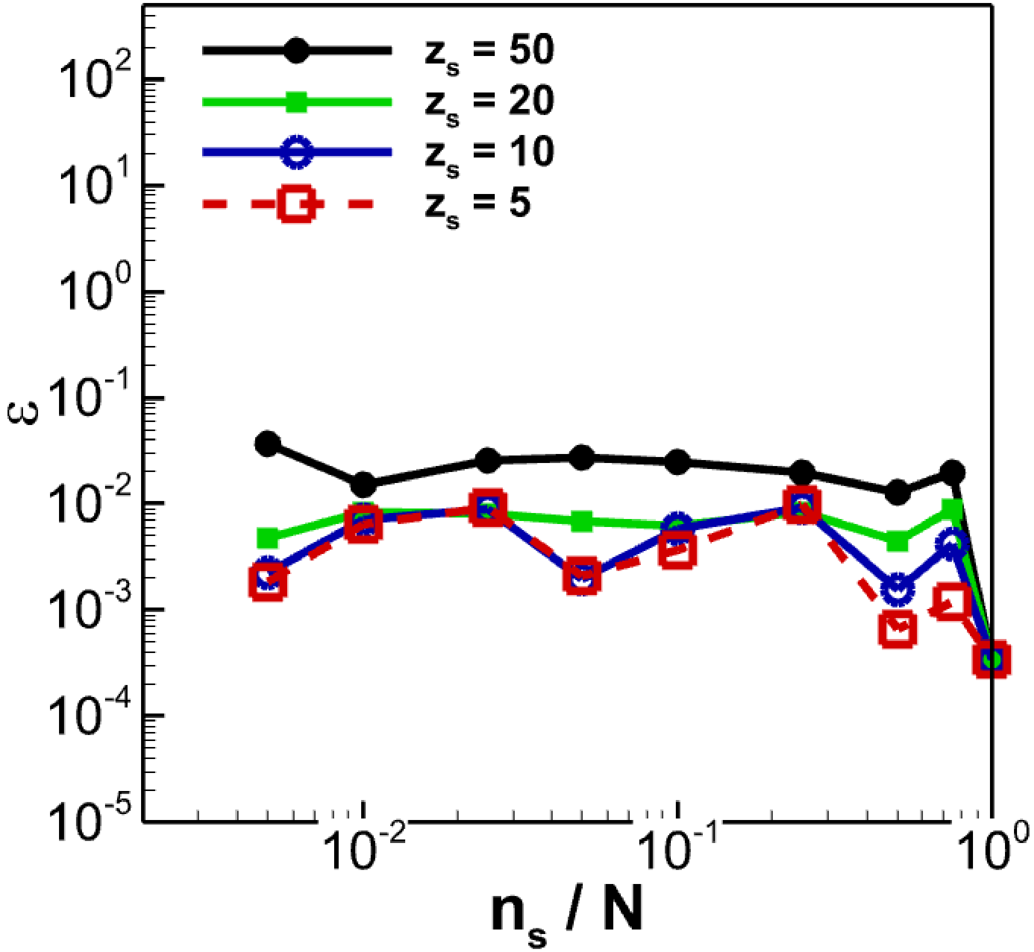


Recommended Metrics for Performance Assessment – Accuracy

Huang and Duraisamy, https://arxiv.org/abs/2301.09006

- **Accuracy should be evaluated over the hyper-parameters:**

$$\varepsilon = \sum_{n=1}^{N_t} \frac{\left\| \mathbf{q}_{FOM}^{n} - \mathbf{q}_{ROM}^{n} \right\|_2}{\left\| \mathbf{q}_{FOM}^{n} \right\|_2}$$

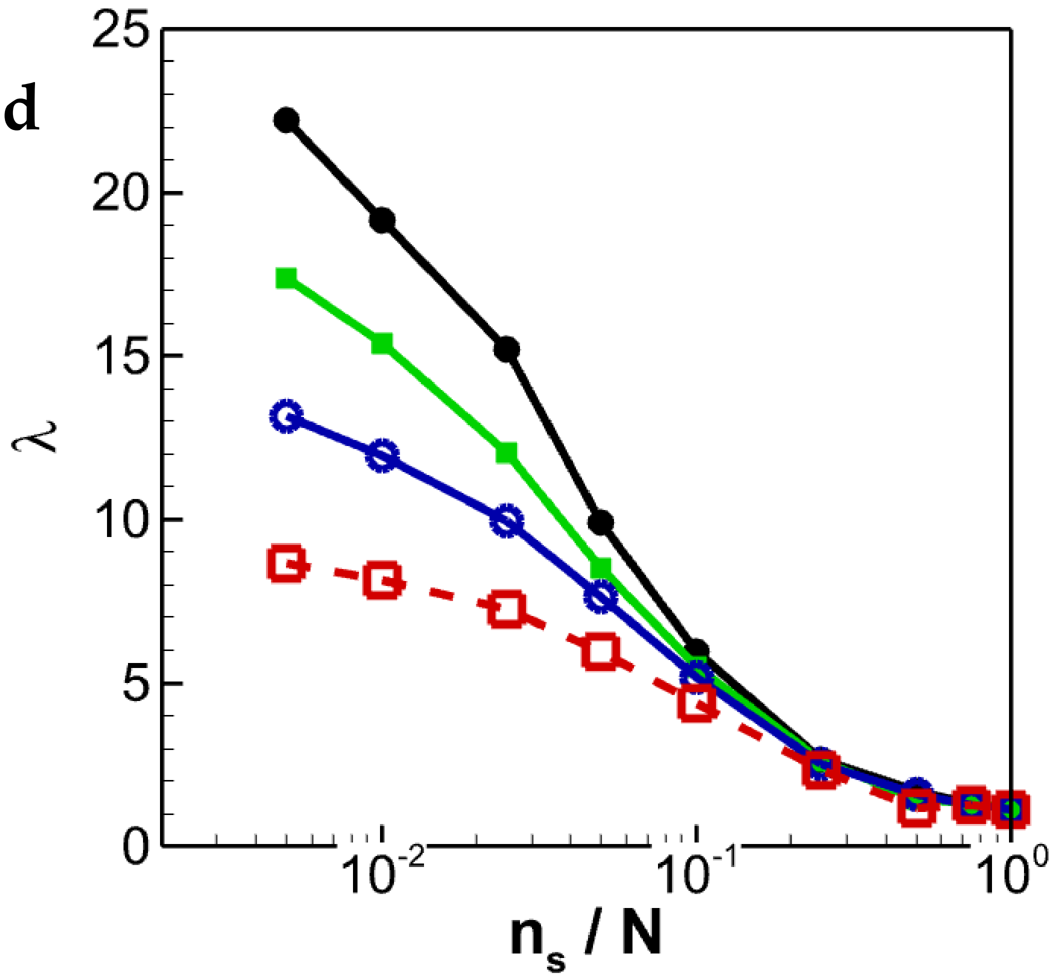


Recommended Metrics for Performance Assessment – Online Cost

Huang and Duraisamy, https://arxiv.org/abs/2301.09006

- **Online cost should be evaluated over the hyper-parameters:**

$$\lambda = \frac{(\text{CPU Hours})_{FOM}}{(\text{CPU Hours})_{ROM}}$$



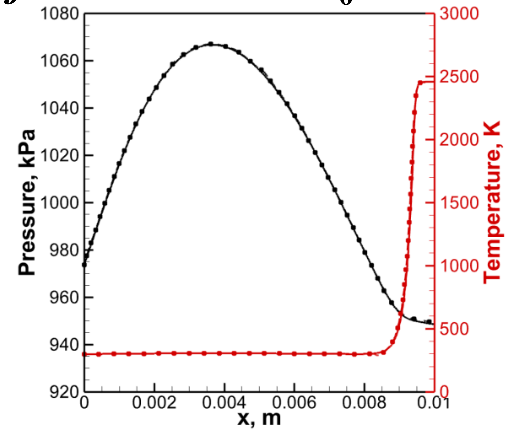
Recommended **Metrics for Performance Assessment** – Offline Cost

$$\gamma = \frac{\text{Number of training snapshots}}{\text{Number of testing snapshots}}$$

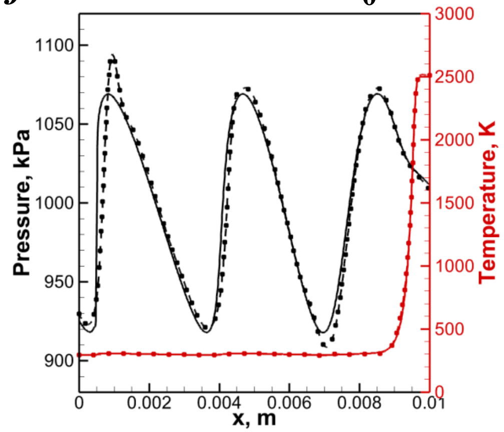
$$\left(e.g. = \frac{10}{4500} \approx 0.2\% \right)$$

Additional **Metrics for Performance Assessment** – Parametric Predictive Capability

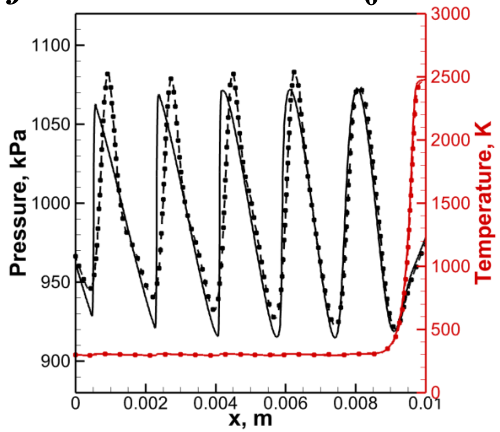
f = 25kHz and A_0 = 0.10



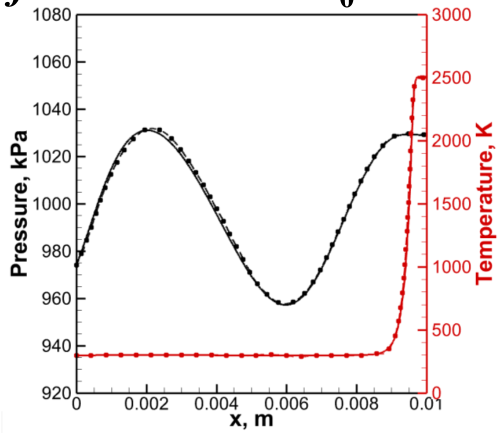
f = 100kHz and A_0 = 0.10



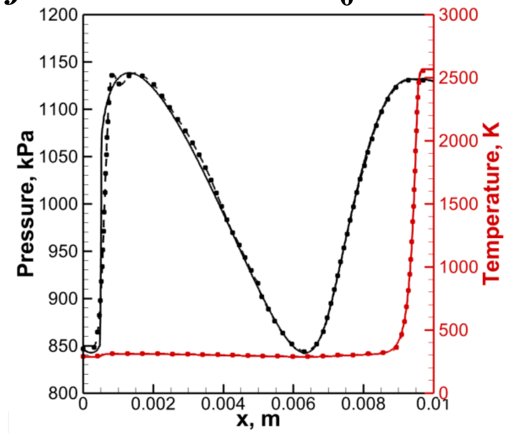
f = 200kHz and A_0 = 0.10

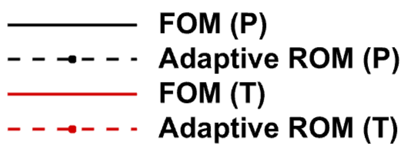


f = 50kHz and A_0 = 0.05



f = 50kHz and A_0 = 0.20





Thank You!

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