



# Robust Reduced Order Modeling for Complex Multi-scale Problems

Karthik Duraisamy



[caslab.engin.umich.edu](http://caslab.engin.umich.edu) & [afcoe.engin.umich.edu](http://afcoe.engin.umich.edu)



Cheng Huang



Chris Wentland



Nicholas Arnold-Medabalimi

+ Center of Excellence Team ([afcoe.engin.umich.edu](http://afcoe.engin.umich.edu))

---

# Acknowledgment

# Multilevel Autoencoder networks

## Introduction

### SP-LSVT ROMs

- Formulation
- Results

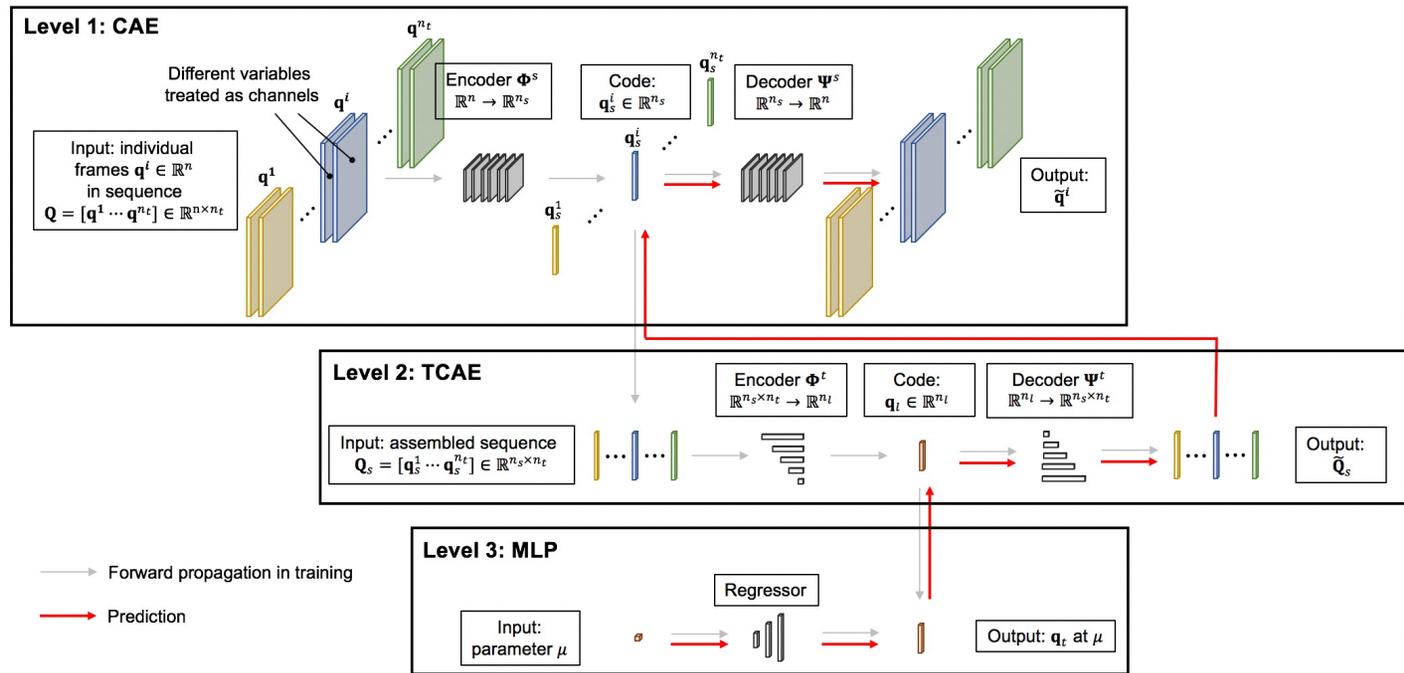
### Adaptive Basis

- Formulation
- Results

### ROM Networks

- Formulation
- Results

## Summary



J Xu, K Duraisamy [Multi-level convolutional autoencoder networks for parametric prediction of spatio-temporal dynamics](#) Computer Methods in Applied Mechanics and Engineering 372, 2019

# Math + physics + structure for Learning

Introduction

SP-LSVT ROMs

- Formulation
- Results

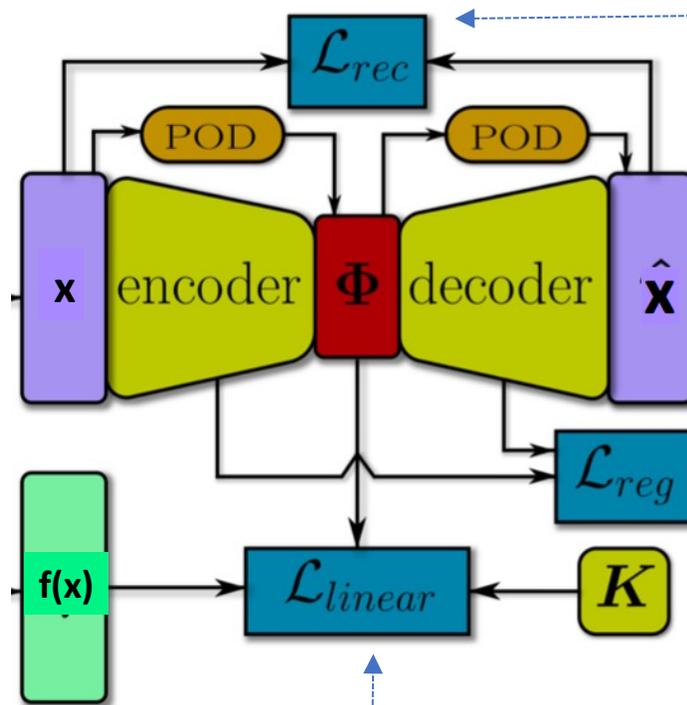
Adaptive Basis

- Formulation
- Results

ROM Networks

- Formulation
- Results

Summary



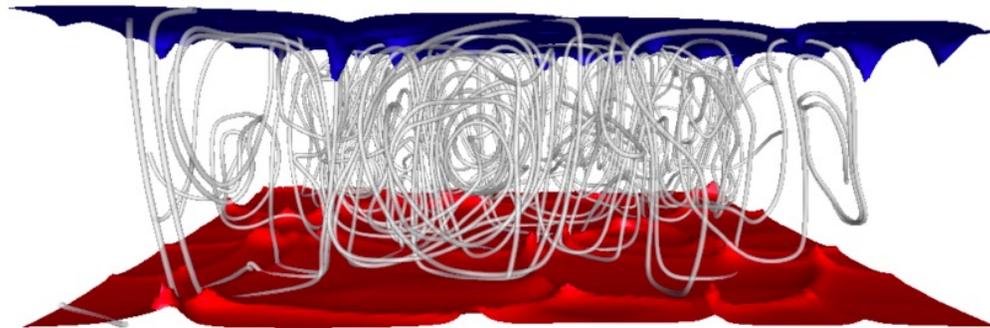
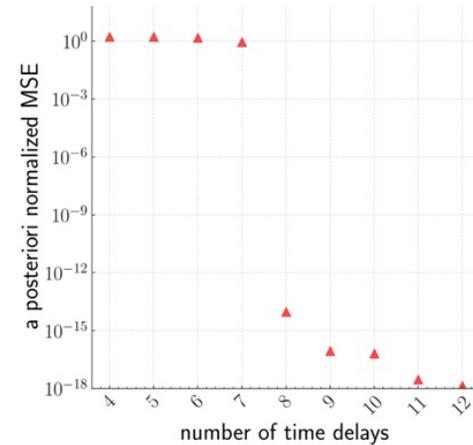
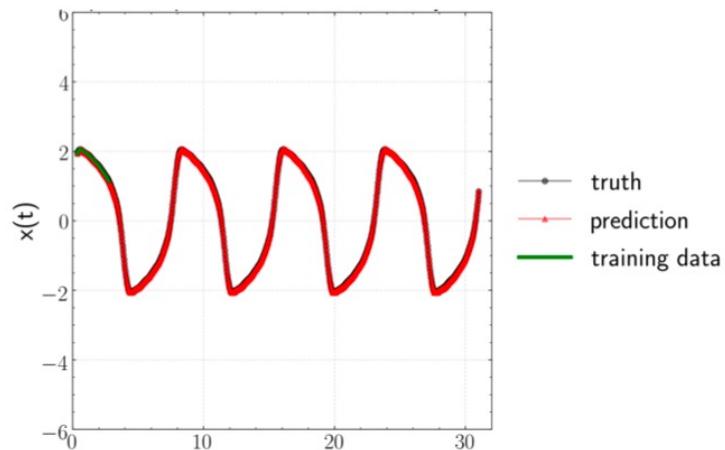
$$\frac{1}{M} \sum_{i=1}^M \|\Psi(\Phi(\mathbf{x}_i)) - \mathbf{x}_i\|^2$$

$$\begin{aligned} \Phi(\mathbf{x}) &= \Phi_{dmd}(\mathbf{x}) + \Phi_{nn}(\mathbf{x}), \\ \Psi(\Phi) &= \Psi_{dmd}(\Phi(\mathbf{x})) + \Psi_{nn}(\Phi(\mathbf{x})) \end{aligned}$$

$$\frac{1}{M} \sum_{i=1}^M \|\mathbf{f}(\mathbf{x}_i) \cdot \nabla_{\mathbf{x}} \Phi(\mathbf{x}_i) - \Phi(\mathbf{x}_i) \mathbf{K}\|^2$$

Pan, S. & Duraisamy, K., *Physics-Informed Probabilistic Learning of Linear Embeddings of Non-linear Dynamics With Guaranteed Stability*, SIAM J. of Applied Dynamical Systems, 2020.

## Power of linear embedding $\hat{\mathbf{x}}_{j+1} = \mathbf{W}_0\mathbf{x}_j + \mathbf{W}_1\mathbf{x}_{j-1} + \dots + \mathbf{W}_L\mathbf{x}_{j-L},$



On the Structure of Time-delay Embedding in Linear Models of Non-linear Dynamical Systems  
Pan & Duraisamy, Chaos 2020

Introduction

SP-LSVT ROMs

- Formulation
- Results

Adaptive Basis

- Formulation
- Results

ROM Networks

- Formulation
- Results

Non-Intrusive  
ROMs

- Formulation
- Results

Summary

## Metrics for Reduced order models

- Accuracy
- Robustness
- Realizability
- `True' Predictivity\*
- Efficiency\*
- Time & complexity of development\*
- Portability\*
- Data requirements
  - ➔ Type of data
  - ➔ Amount of data

\* Non-intrusive ROMs clearly win here

\* Adaptive intrusive ROMs

# A few things to take home

Introduction

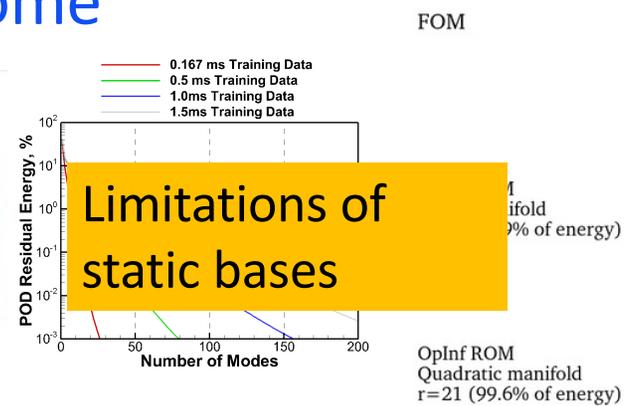
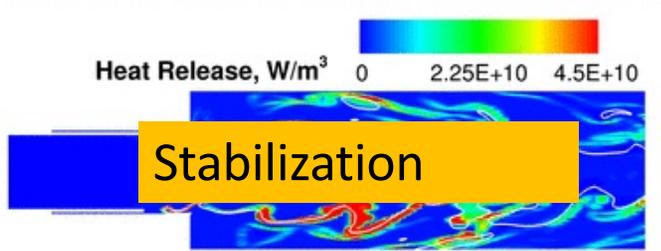
- SP-LSVT ROMs
  - Formulation
  - Results

- Adaptive Basis
  - Formulation
  - Results

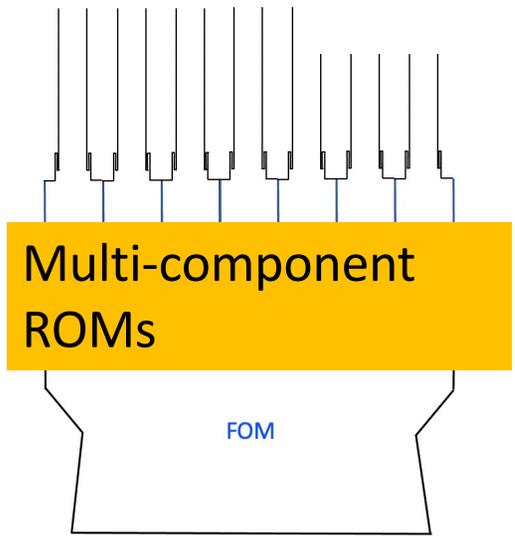
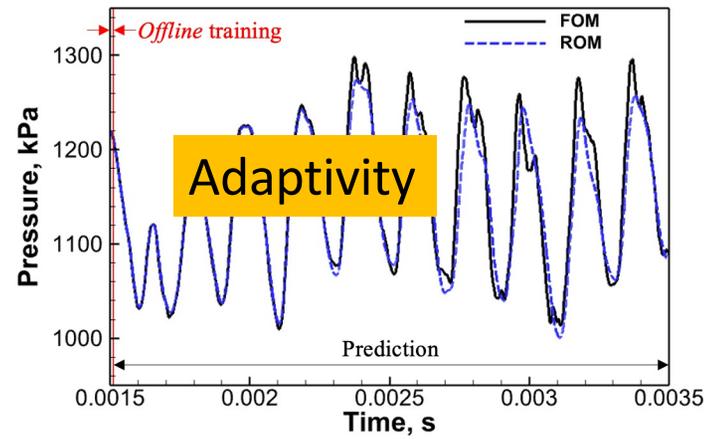
- ROM Networks
  - Formulation
  - Results

- Non-Intrusive ROMs
  - Formulation
  - Results

Summary



Non-intrusive ROMs



## Projection-based ROMs

Full order model

$$\frac{d\mathbf{q}}{dt} = \mathbf{f}(\mathbf{q}, t), \quad \mathbf{q}(0) = \mathbf{q}_0,$$

define a trial basis  $\mathbf{V} \in \mathbb{R}^{n \times k}$  that spans a subspace  $\mathcal{V} \subset \mathbb{R}^n$ .

$$\mathbf{q} = \mathbf{V}\mathbf{q}_r + \mathbf{V}^\perp\mathbf{q}_p.$$

Approximate

$$\tilde{\mathbf{q}} = \mathbf{V}\mathbf{q}_r$$

Let's define a test basis  $\mathbf{W}$  and project the equation onto the test subspace,

Project

$$\mathbf{W}^T \mathbf{V} \frac{d\mathbf{q}_r(t)}{dt} = \mathbf{W}^T \mathbf{f}(\mathbf{V}\mathbf{q}_r(t), t), \quad \mathbf{W}^T \mathbf{V}\mathbf{q}_r(0) = \mathbf{W}^T \mathbf{q}_0$$

ROM

$$\frac{d\mathbf{q}_r(t)}{dt} = [\mathbf{W}^T \mathbf{V}]^{-1} \mathbf{W}^T \mathbf{f}(\mathbf{V}\mathbf{q}_r(t), t), \quad \mathbf{q}_r(0) = [\mathbf{W}^T \mathbf{V}]^{-1} \mathbf{W}^T \mathbf{q}_0.$$

Equivalent  
FOM

$$\frac{d\tilde{\mathbf{q}}(t)}{dt} = \mathbf{V} [\mathbf{W}^T \mathbf{V}]^{-1} \mathbf{W}^T \mathbf{f}(\tilde{\mathbf{q}}(t), t), \quad \tilde{\mathbf{q}}(0) = \mathbf{V} [\mathbf{W}^T \mathbf{V}]^{-1} \mathbf{W}^T \mathbf{q}_0.$$

## Galerkin ROMs

Full Order Model  $\frac{d\mathbf{q}}{dt} = \mathbf{f}(\mathbf{q}, t), \quad \mathbf{q}(0) = \mathbf{q}_0, \quad \mathbf{q} : [0, T] \rightarrow \mathbb{R}^N$

define a trial basis  $\mathbf{V} \in \mathbb{R}^{n \times k}$  that spans a subspace  $\mathcal{V} \subset \mathbb{R}^n$ .

$$\mathbf{q} = \mathbf{V}\mathbf{q}_r + \mathbf{V}^\perp\mathbf{q}_p.$$

Approximate

$$\tilde{\mathbf{q}} = \mathbf{V}\mathbf{q}_r$$

Substitute

$$\frac{d\mathbf{V}\mathbf{q}_r(t)}{dt} = \mathbf{f}(\mathbf{V}\mathbf{q}_r(t), t), \quad \mathbf{V}\mathbf{q}_r(0) = \mathbf{q}_0$$

Project

$$\frac{d\mathbf{q}_r(t)}{dt} = \mathbf{V}^T \mathbf{f}(\mathbf{V}\mathbf{q}_r(t), t), \quad \mathbf{q}_r(0) = \mathbf{V}^T \mathbf{q}_0.$$

## Error Transport

$$\begin{aligned}\boldsymbol{\epsilon}(t) &= \mathbf{q}(t) - \tilde{\mathbf{q}}(t) \\ &= \mathbf{q}(t) - \mathbf{V}\mathbf{q}_r(t) \\ &= \mathbf{q}(t) - \boldsymbol{\Pi}\mathbf{q}(t) + \boldsymbol{\Pi}\mathbf{q}(t) - \mathbf{V}\mathbf{q}_r(t) \\ &= [(\mathbf{I} - \boldsymbol{\Pi})\mathbf{q}(t)] + [\boldsymbol{\Pi}\mathbf{q}(t) - \mathbf{V}\mathbf{q}_r(t)] \\ &= \boldsymbol{\epsilon}_\Pi(t) + \boldsymbol{\epsilon}_\parallel(t).\end{aligned}$$

$$\frac{d\boldsymbol{\epsilon}_\parallel}{dt} = \boldsymbol{\Pi} [\mathbf{f}(\mathbf{q}(t), t) - \mathbf{f}(\tilde{\mathbf{q}}(t), t)]$$

# Stability

Let's consider an autonomous linear system  $\mathbf{f}(\mathbf{q}(t), t) = \mathbf{A}\mathbf{q}(t)$ , then

$$\frac{d\boldsymbol{\epsilon}_{\parallel}}{dt} = \boldsymbol{\Pi}\mathbf{A}\boldsymbol{\epsilon}_{\parallel}(t) + \boldsymbol{\Pi}\mathbf{A}\boldsymbol{\epsilon}_{\Pi}(t).$$

$$\begin{aligned} \boldsymbol{\epsilon}_{\parallel}^T \frac{d\boldsymbol{\epsilon}_{\parallel}}{dt} &= \boldsymbol{\epsilon}_{\parallel}^T \boldsymbol{\Pi}\mathbf{A}\boldsymbol{\epsilon}_{\parallel} + \boldsymbol{\epsilon}_{\parallel}^T \boldsymbol{\Pi}\mathbf{A}\boldsymbol{\epsilon}_{\Pi} \\ \frac{1}{2} \frac{d\boldsymbol{\epsilon}_{\parallel}^T \boldsymbol{\epsilon}_{\parallel}}{dt} &= \frac{1}{2} \boldsymbol{\epsilon}_{\parallel}^T [\boldsymbol{\Pi}\mathbf{A} + [\boldsymbol{\Pi}\mathbf{A}]^T] \boldsymbol{\epsilon}_{\parallel} + \boldsymbol{\epsilon}_{\parallel}^T \boldsymbol{\Pi}\mathbf{A}\boldsymbol{\epsilon}_{\perp} \end{aligned}$$

we get the necessary condition <sup>2</sup>, that  $\boldsymbol{\Pi}\mathbf{A} + [\boldsymbol{\Pi}\mathbf{A}]^T$  should be negative definite. Additionally, the interaction between the parallel and orthogonal errors may also affect stability in a profound manner.

In Galerkin ROMs, we do not have a great degree of control over  $\boldsymbol{\Pi}$ . Petrov Galerkin methods give us additional control knobs to improve both accuracy and stability.

## Galerkin & LSPG

FOM

$$\mathbf{q}^n = \mathbf{q}^{n-1} + \Delta t \mathbf{A} \mathbf{q}^n$$

Galerkin ROM

$$[\mathbf{I} - \Delta t \mathbf{V}^T \mathbf{A} \mathbf{V}] \mathbf{q}_r^n = [\mathbf{I} - \Delta t \mathbf{V}^T \mathbf{A} \mathbf{V}] \mathbf{q}_r^{n-1}$$

Least squares projection

$$\min_{\mathbf{q}_r^n} \|\mathbf{V} \mathbf{q}_r^n - \mathbf{V} \mathbf{q}_r^{n-1} - \Delta t \mathbf{A} \mathbf{V} \mathbf{q}_r^n\|_2^2$$

Farhat and co-workers,  
circa 2010

LSPG ROM

$$[\mathbf{I} - \Delta t \mathbf{V}^T \mathbf{A} \mathbf{V} - \Delta t \mathbf{V}^T \mathbf{A}^T \mathbf{V} + \Delta t^2 \mathbf{V}^T \mathbf{A}^T \mathbf{A} \mathbf{V}] \mathbf{q}_r^n = [\mathbf{I} - \Delta t \mathbf{V}^T \mathbf{A}^T \mathbf{V}] \mathbf{q}_r^{n-1}$$

## Linear Manifold ROMs

Continuous  
FOM

$$\frac{d\mathbf{q}}{dt} = \mathbf{f}(\mathbf{q}, t), \quad \mathbf{q}(0) = \mathbf{q}_0, \quad \mathbf{q} : [0, T] \rightarrow \mathbb{R}^N$$

Introduction

SP-LSVT ROMs

- Formulation
- Results

Discrete  
FOM

$$\mathbf{r}(\mathbf{q}^n) \triangleq \mathbf{q}^n + \sum_{j=1}^l \alpha_j \mathbf{q}^{n-j} - \Delta t \beta_0 \mathbf{f}(\mathbf{q}^n, t^n) - \Delta t \sum_{j=1}^l \beta_j \mathbf{f}(\mathbf{q}^{n-j}, t^{n-j})$$

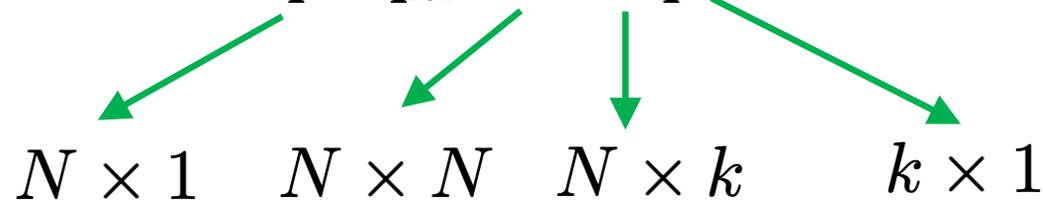
Adaptive Basis

- Formulation
- Results

ROM Networks

- Formulation
- Results

Reduced  
representation  
in Linear  
subspace

$$\tilde{\mathbf{q}} = \mathbf{q}_{\text{ref}} + \mathbf{P}^{-1} \mathbf{V} \mathbf{q}_r$$


$N \times 1$      $N \times N$      $N \times k$      $k \times 1$

Summary

## Linear Stability : 1/2

Continuous FOM

$$\frac{d\mathbf{q}}{dt} = \mathbf{J}\mathbf{q}, \quad \mathbf{q}(0) = \mathbf{q}_0,$$

Discrete FOM

$$(\mathbf{I} - \Delta t \mathbf{J}) \mathbf{q}^n = \mathbf{q}^{n-1}, \quad \mathbf{q}^0 = \mathbf{q}_0$$

Decomposition

$$\tilde{\mathbf{q}}(t) \triangleq \mathbf{V} \mathbf{q}_r(t), \quad \text{where } \mathbf{V} \in \mathbb{R}^{N \times k} \text{ and } \mathbf{q}_r \in \mathbb{R}^k$$

**Theorem 1 :** *If the Discrete FOM above is asymptotically stable in the sense of  $\|(\mathbf{I} - \Delta t \mathbf{J})^{-1}\|_2 \leq 1$ , then the Backward Euler Galerkin ROM is also asymptotically stable if  $\lambda_n(\mathbf{I} - 0.5\Delta t(\mathbf{J} + \mathbf{J}^T)) \geq 1$*

[Model Reduction for Multi-Scale Transport Problems using Structure-Preserving Least-Squares Projections with Variable Transformation](#) C Huang, C Wentland, K Duraisamy, C Merkle, JCP 2021.

Introduction

SP-LSVT ROMs

- Formulation
- Results

Adaptive Basis

- Formulation
- Results

ROM Networks

- Formulation
- Results

Summary

## Linear Stability : 2/2

Continuous FOM

$$\frac{d\mathbf{q}}{dt} = \mathbf{J}\mathbf{q}, \quad \mathbf{q}(0) = \mathbf{q}_0,$$

Discrete FOM

$$(\mathbf{I} - \Delta t \mathbf{J})\mathbf{q}^n = \mathbf{q}^{n-1}, \quad \mathbf{q}^0 = \mathbf{q}_0$$

Decomposition

$$\tilde{\mathbf{q}}(t) \triangleq \mathbf{V}\mathbf{q}_r(t), \quad \text{where } \mathbf{V} \in \mathbb{R}^{N \times k} \text{ and } \mathbf{q}_r \in \mathbb{R}^k$$

**Theorem 2 :** *If the Discrete FOM above is asymptotically stable in the sense of  $\|(\mathbf{I} - \Delta t \mathbf{J})^{-1}\|_2 \leq 1$ , then the associated LSPG ROM is also asymptotically stable with no further assumptions required.*

[Model Reduction for Multi-Scale Transport Problems using Structure-Preserving Least-Squares Projections with Variable Transformation](#) C Huang, C Wentland, K Duraisamy, C Merkle, JCP 2021.

Introduction

SP-LSVT ROMs

- Formulation
- Results

Adaptive Basis

- Formulation
- Results

ROM Networks

- Formulation
- Results

Summary

## Linear Manifold Projection-based ROMs

$$\frac{d\mathbf{q}}{dt} = \mathbf{f}(\mathbf{q}, t), \quad \mathbf{q}(0) = \mathbf{q}_0, \quad \mathbf{q} : [0, T] \rightarrow \mathbb{R}^N$$

$$\mathbf{r}(\mathbf{q}^n) \triangleq \mathbf{q}^n + \sum_{j=1}^l \alpha_j \mathbf{q}^{n-j} - \Delta t \beta_0 \mathbf{f}(\mathbf{q}^n, t^n) - \Delta t \sum_{j=1}^l \beta_j \mathbf{f}(\mathbf{q}^{n-j}, t^{n-j})$$

$$\mathcal{V} \triangleq \text{Range}(\mathbf{P}^{-1} \mathbf{V})$$

Projection

$$\frac{d\mathbf{q}_r}{dt} = \mathbf{V}^T \mathbf{P} \mathbf{f}(\tilde{\mathbf{q}}, t) \quad \tilde{\mathbf{q}}^n \triangleq \arg \min_{\tilde{\mathbf{q}}^n \in \text{Range}(\mathbf{V})} \|\mathbf{P} \mathbf{r}(\tilde{\mathbf{q}}^n)\|_2^2$$

Galerkin

Least Squares

### Introduction

#### SP-LSVT ROMs

- Formulation
- Results

#### Adaptive Basis

- Formulation
- Results

#### ROM Networks

- Formulation
- Results

### Summary

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

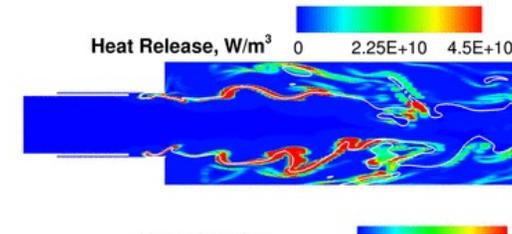
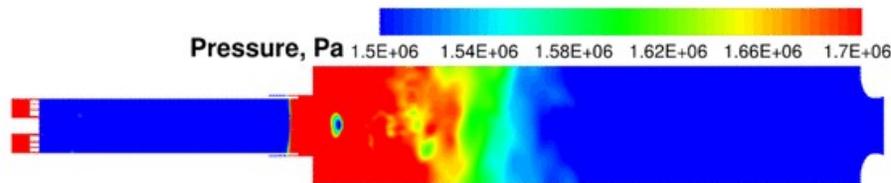
- Non-linear, Multi-scale multi-physics interactions : acoustics, flow & reaction
- Flow – Large coherent structures + small shear layer dynamics
- Reaction – Highly intensive, distributed & intermittent thin flame
- High sensitivity to parameter changes

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

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

**Highly nonlinear and stiff source term :**

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



Introduction

SP-LSVT ROMs

- Formulation
- Results

Adaptive Basis

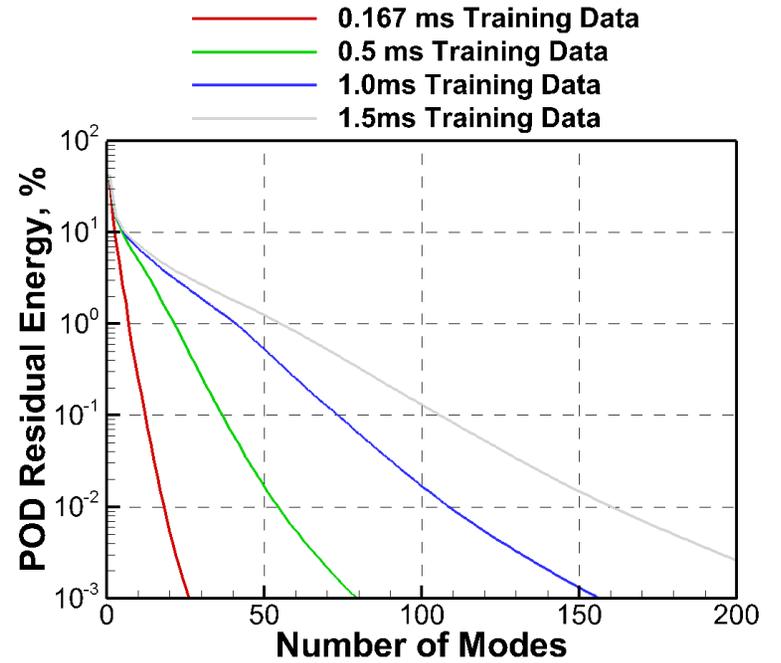
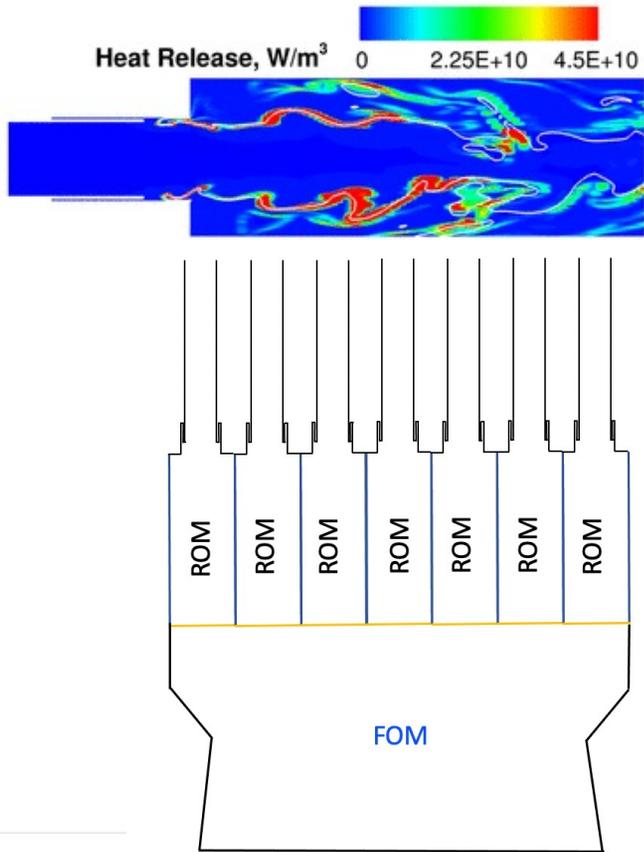
- Formulation
- Results

ROM Networks

- Formulation
- Results

Summary

# 3 Things to take home



Key Enabler : Adaptivity



Introduction

SP-LSVT ROMs

- Formulation
- Results

Adaptive Basis

- Formulation
- Results

ROM Networks

- Formulation
- Results

Summary

## Part 1

# Robustness & Accuracy

*[Model Reduction for Multi-Scale Transport Problems using Structure-Preserving Least-Squares Projections with Variable Transformation](#) C Huang, C Wentland, K Duraisamy, JCP, 2021*



## Discretely-consistent Petrov-Galerkin ROMs with Variable Transformation (1/3)

Conserved variables

### Conservative Equations

$$\frac{\mathbf{q}^{n+1} - \mathbf{q}^n}{\Delta t} = \mathbf{f}(\mathbf{q}^{n+1})$$

### Pseudo time stepping

$$\delta \mathbf{q} = \Gamma \delta \mathbf{s}$$

$$\Gamma^{p-1} \frac{\mathbf{s}^p - \mathbf{s}^{p-1}}{\Delta \tau} + \frac{\mathbf{q}^p - \mathbf{q}^n}{\Delta t} = \mathbf{f}(\mathbf{q}^p)$$

Primitive variables

### Fully Discrete Residual

$$\mathbf{r}_s(\mathbf{s}^p) \triangleq \left[ \left( \frac{\Delta t}{\Delta \tau} + 1 \right) \mathbf{I} - \Delta t \mathbf{J}^{p-1} \right] \Gamma^{p-1} (\mathbf{s}^p - \mathbf{s}^{p-1}) + (\mathbf{q}^{p-1} - \mathbf{q}^n) - \Delta t \mathbf{f}(\mathbf{q}^{p-1})$$

Discrete equations

$$\mathbf{r}_s(\mathbf{s}^p) \triangleq \left[ \left( \frac{\Delta t}{\Delta \tau} + 1 \right) \mathbf{I} - \Delta t \mathbf{J}^{p-1} \right] \Gamma^{p-1} (\mathbf{s}^p - \mathbf{s}^{p-1}) + (\mathbf{q}^{p-1} - \mathbf{q}^n) - \Delta t \mathbf{f}(\mathbf{q}^{p-1})$$

Decomposition

$$\tilde{\mathbf{s}} \triangleq \bar{\mathbf{s}} + \mathbf{S} \mathbf{V} \mathbf{s}_r$$

Basis  
vectors

Scaling matrix  
for  $\mathbf{s}$

Basis  
coefficients

Discretely-consistent Least-Squares formulation

$$\mathbf{s}_r^p \triangleq \arg \min_{\mathbf{s}_r} \|\mathbf{Q} \mathbf{r}_s(\tilde{\mathbf{s}})\|_2^2$$

Scaling matrix  
for  $\mathbf{q}$

## Discretely-consistent Petrov-Galerkin ROMs with Variable Transformation (3/3)

### Discretely-consistent Least-Squares formulation

$$\mathbf{s}_r^p \triangleq \arg \min_{\mathbf{s}_r} \|\mathbf{Q}\mathbf{r}_s(\tilde{\mathbf{s}})\|_2^2$$

### Test basis

$$\mathbf{W}^{p-1} \triangleq \mathbf{Q} \left[ \left( \frac{\Delta t}{\Delta \tau} + 1 \right) \mathbf{I} - \Delta t \mathbf{J}^{p-1} \right] \Gamma^{p-1} \mathbf{S} \mathbf{V}$$

### ROM

$$[\mathbf{W}^{p-1}]^T \mathbf{W}^{p-1} (\mathbf{s}_r^p - \mathbf{s}_r^{p-1}) = -[\mathbf{W}^{p-1}]^T \mathbf{Q}\mathbf{r}_q^{p-1}$$

Discretely-consistent, symmetrized, (globally)stable, conservative

# Hyper-reduction

Re-define discrete least square formulation based on  $N_s$  samples

$$[\mathbf{W}^{p-1}]^T \mathbf{W}^{p-1} (\mathbf{s}_r^p - \mathbf{s}_r^{p-1}) = -[\mathbf{W}^{p-1}]^T [\mathbf{P}\mathbf{U}]^+ \mathbf{P}\mathbf{Q}\mathbf{r}_q^{p-1}$$

$$[\mathbf{P}\mathbf{U}]^+ \mathbf{P}\mathbf{Q} \left[ \left( \frac{\Delta t}{\Delta \tau} + 1 \right) \mathbf{I} - \Delta t \mathbf{J}^{p-1} \right] \Gamma^{p-1} \mathbf{S}\mathbf{V}$$

$N_s \times k$

$k \times N_s$   
precomputed

$$\mathbf{P}\mathbf{Q}((\tilde{\mathbf{q}}^{p-1} - \tilde{\mathbf{q}}^n) - \Delta t \mathbf{f}(\tilde{\mathbf{q}}^{p-1}))$$

$N_s \times 1$

Sampling points  
(QDEIM)

Residual Basis  
(POD)

Introduction

SP-LSVT ROMs

- Formulation
- Results

Adaptive Basis

- Formulation
- Results

ROM Networks

- Formulation
- Results

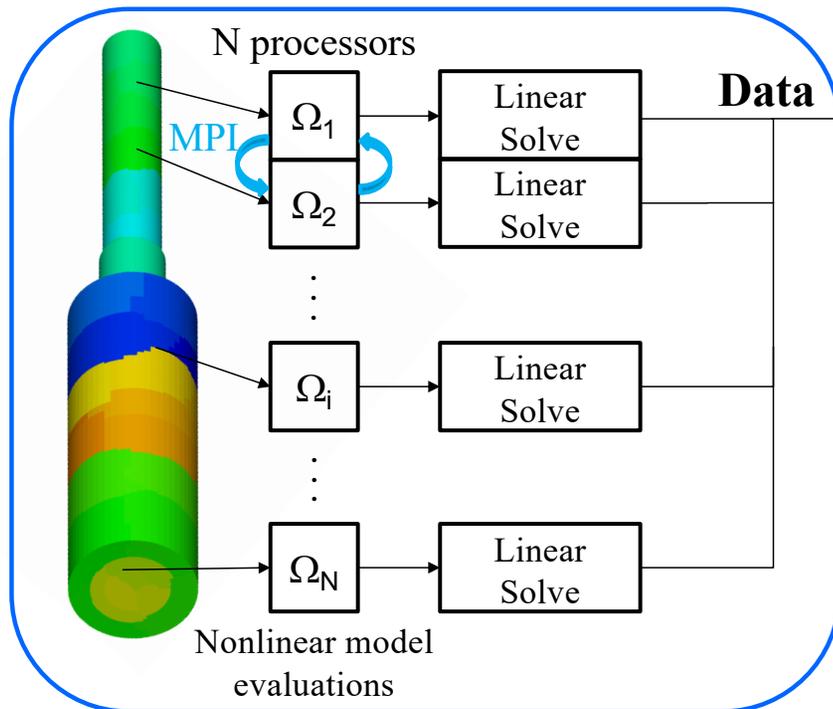
Summary

Preserves discrete consistency, but reduces complexity from  $O(N)$  to  $O(N_s)$

# Parallel Data Processor (PDP) for Large scale ROMs

ROM Software Infrastructure Development → Efficient Data Processor

## CFD Code



## Parallel Data Processor (PDP)

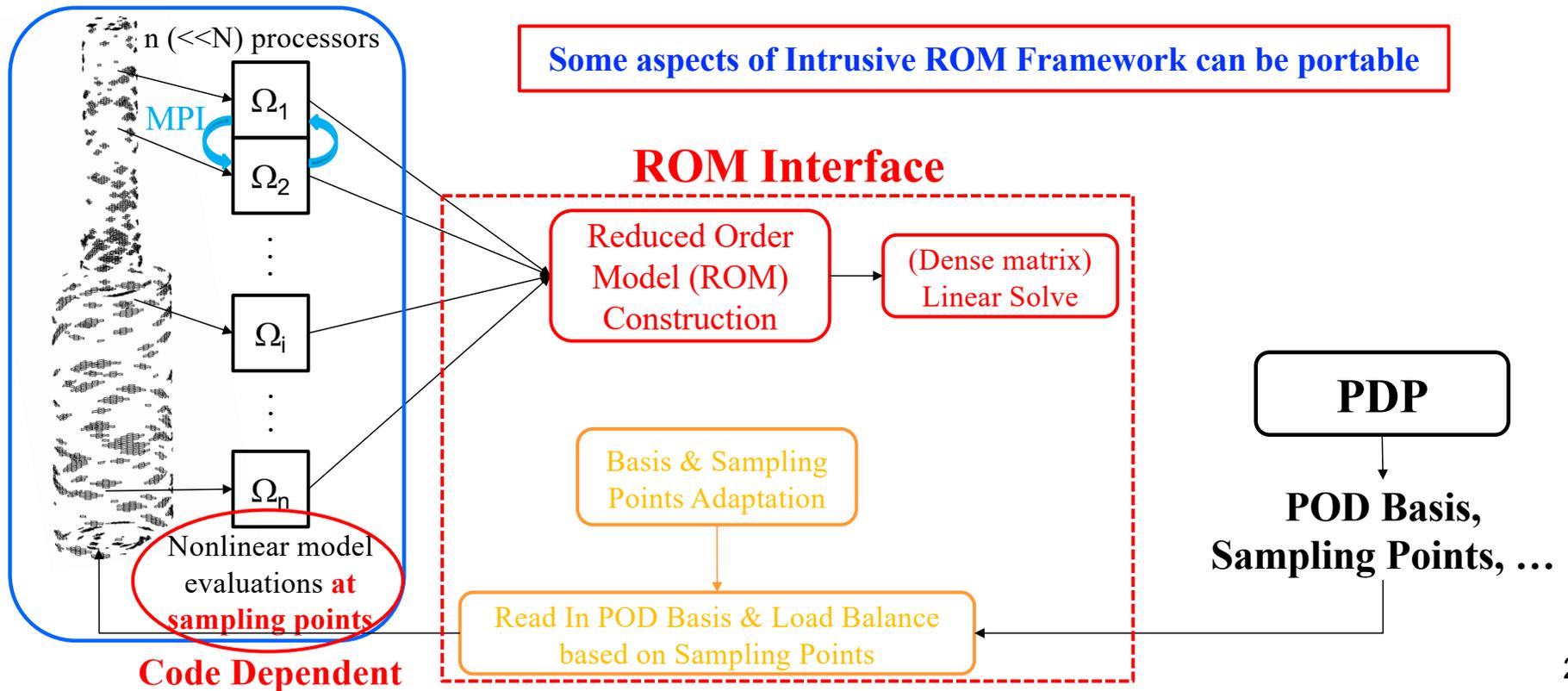
- Parallel toolset for data decomposition (POD/DMD) – shared with Air Force
- Compatible with different data formats
- Efficient basis generation, sparse sampling pre-calculations especially for large scale problems (e.g. **POD with 100M DoFs x 1000 snapshots in less than 30 min**)

POD Basis, Sampling Points, ...

# ROM Interface

ROM Software Infrastructure Development → Portable Parallel Interface

## CFD Code



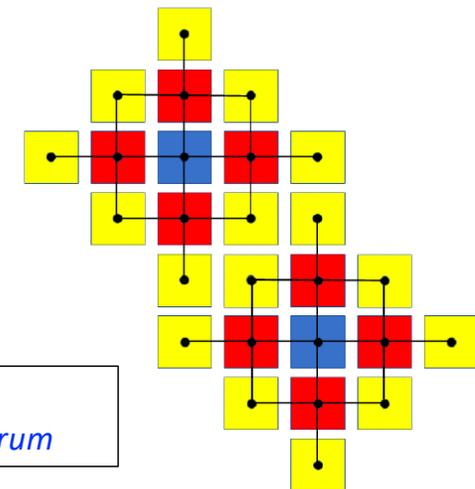
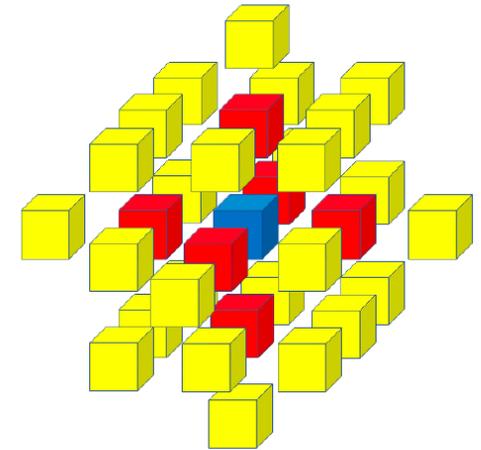
## Further details on sampling

- First  $d$  points selected by QR pivots of data (QDEIM)
- **GappyPOD+R**: randomized oversampling
  - Remaining  $N_s - d$  points are selected randomly
  - Cheap, simple, serial
- **GappyPOD+E**: eigenvector-based oversampling
  - Minimize sampling error at every iteration

$$\left\| [\mathbf{S}_m^T \mathbf{U}]^+ \right\|_2 = \frac{1}{\sigma_{\min}(\mathbf{S}_m^T \mathbf{U})}$$

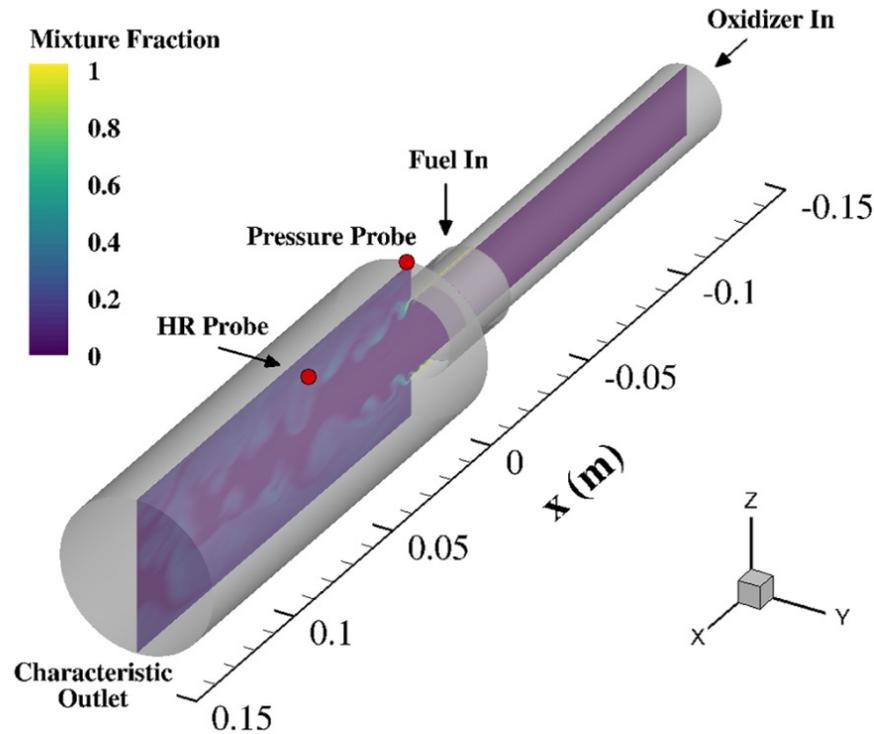
- Sample row of  $\mathbf{U}$  which maximizes update to smallest eigenvalue

$$\lambda_d^{m+1} - \lambda_d^m$$



*Investigation of Sampling Strategies for Reduced-Order Models of Rocket Combustors, CR Wentland, C Huang, K Duraisamy, Proc. AIAA Scitech 2021 Forum*

## Further details on sa



Scalable Projection-Based Reduced-Order Models for Large Multiscale Fluid Systems

, CR Wentland, C Huang, K Duraisamy, AIAA 2023

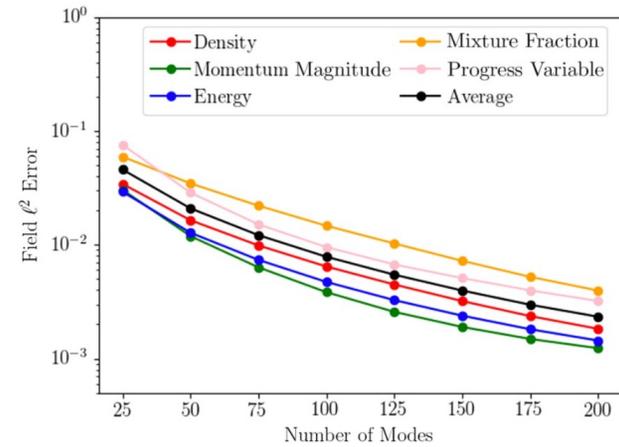


Fig. 19 Conservative variables time-average projection error.

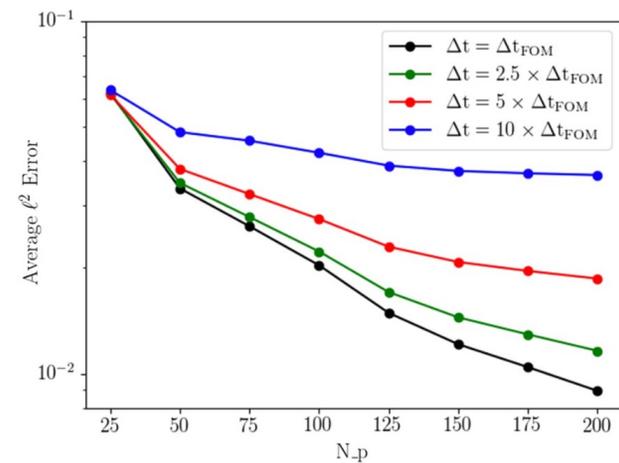
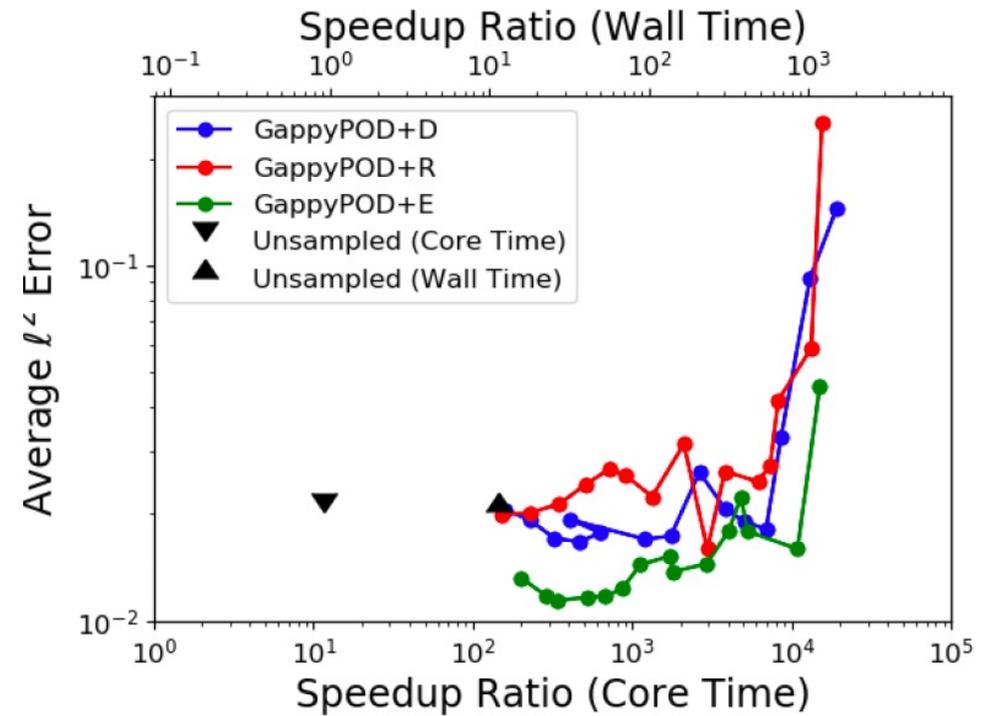
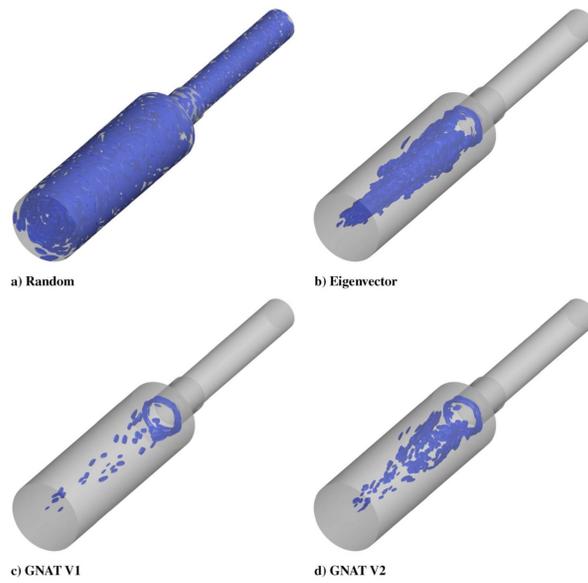


Fig. 20 CVRC unsampled PROM time-average error, various  $\Delta t$ .

## Further details on sampling



*Investigation of Sampling Strategies for Reduced-Order Models of Rocket Combustors, CR Wentland, C Huang, K Duraisamy, Proc. AIAA Scitech 2021 Forum*



UNIVERSITY OF MICHIGAN

Introduction

SP-LSVT ROMs

- Formulation
- Results

Adaptive Basis

- Formulation
- Results

ROM Networks

- Formulation
- Results

Summary

## 3D Truncated CVRC Injector with Downstream Forcing

Oxidizer @  $T = 660\text{K}$

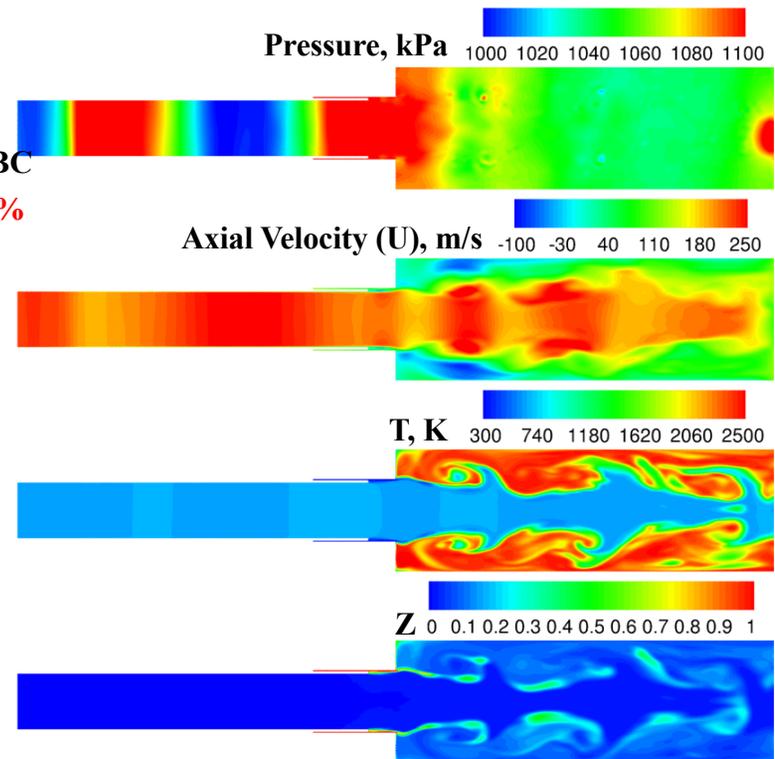
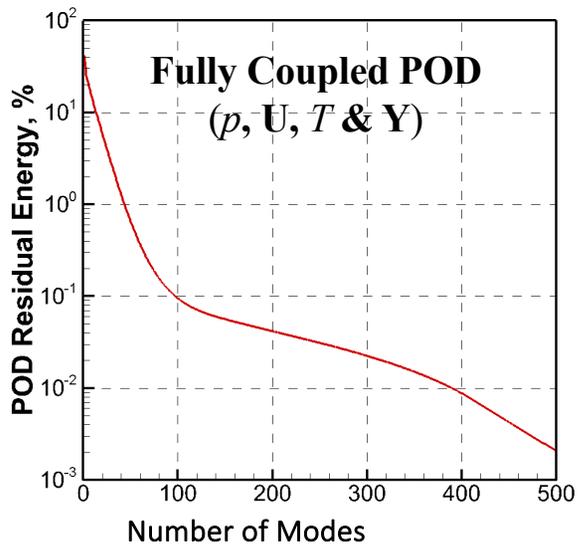
Fuel @  $T = 300\text{K}$

Coarse 3D mesh  
(~ 590K cells)

Characteristic BC

4kHz @ 5%  
amp

Flamelet progress variable model with GRI-1.2 kinetics  
(32 species, 177 reactions)





UNIVERSITY OF MICHIGAN

Introduction

SP-LSVT ROMs

- Formulation
- Results

Adaptive Basis

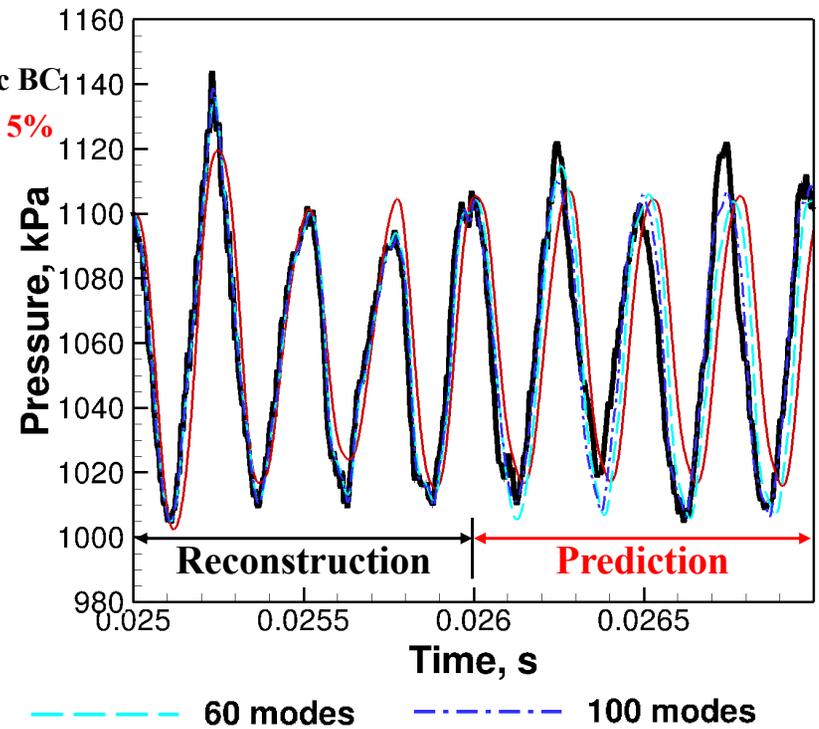
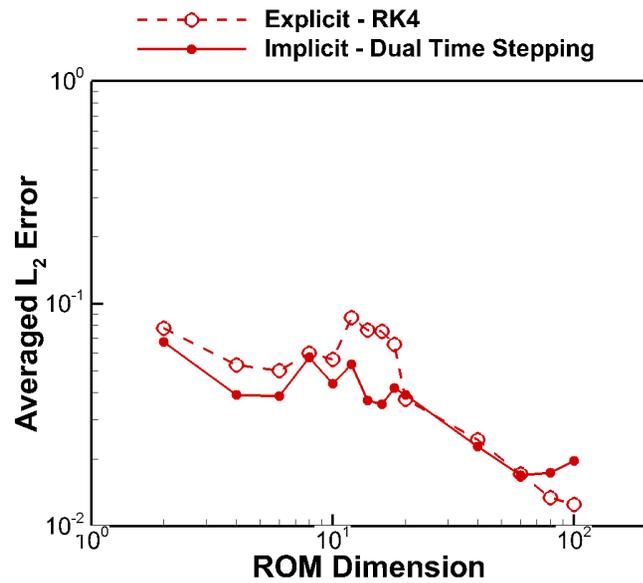
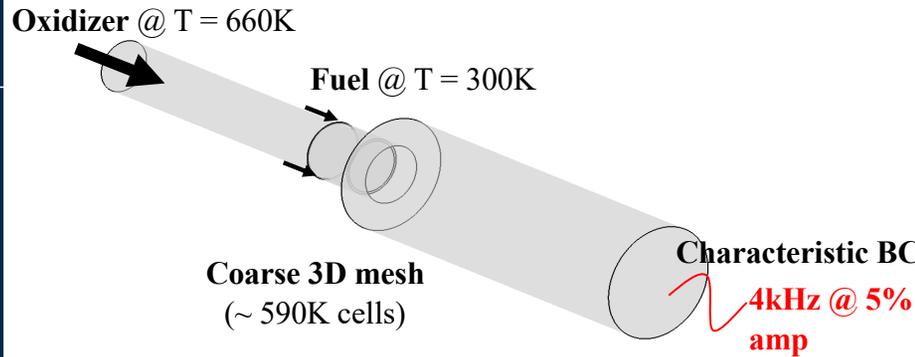
- Formulation
- Results

ROM Networks

- Formulation
- Results

Summary

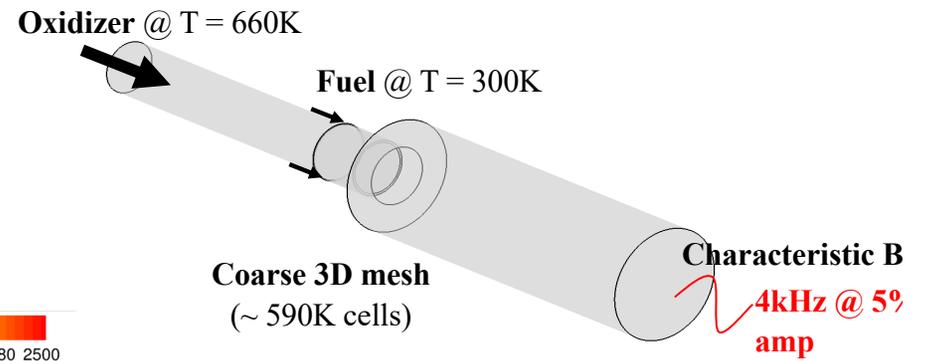
## Model Performance



- Formulation
- Results

- Formulation
- Results

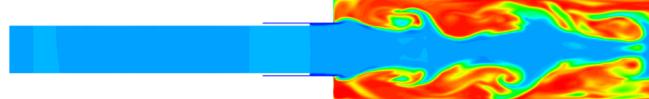
- Formulation
- Results



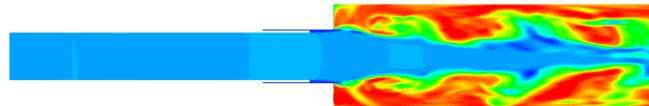
T, K



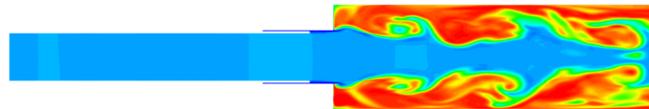
FOM



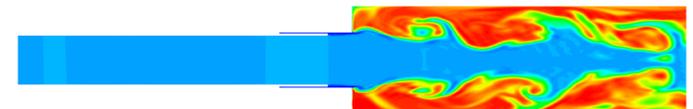
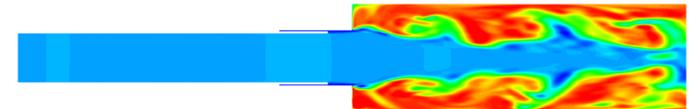
ROM 20  
modes

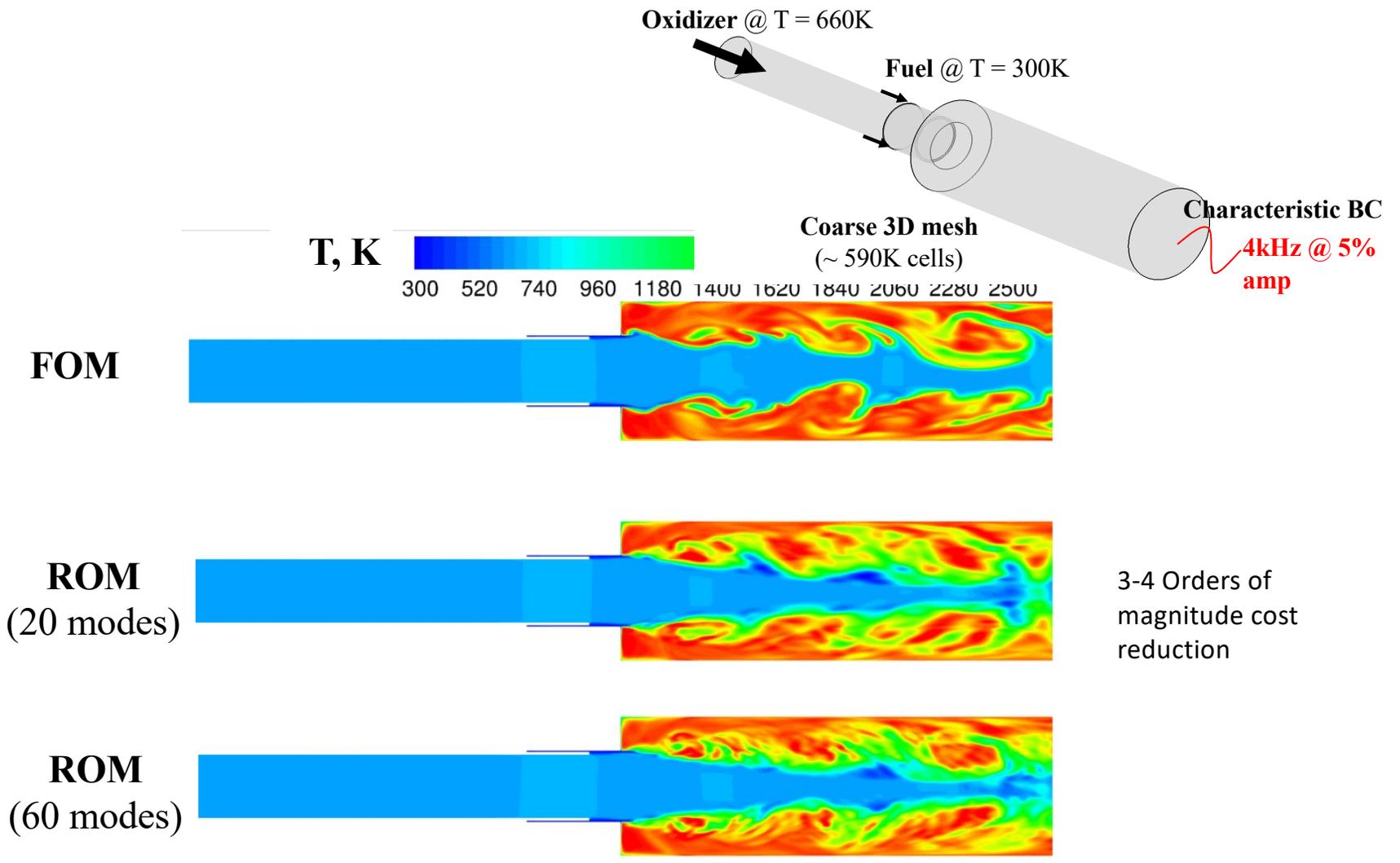


ROM 60  
modes



Projected FOM



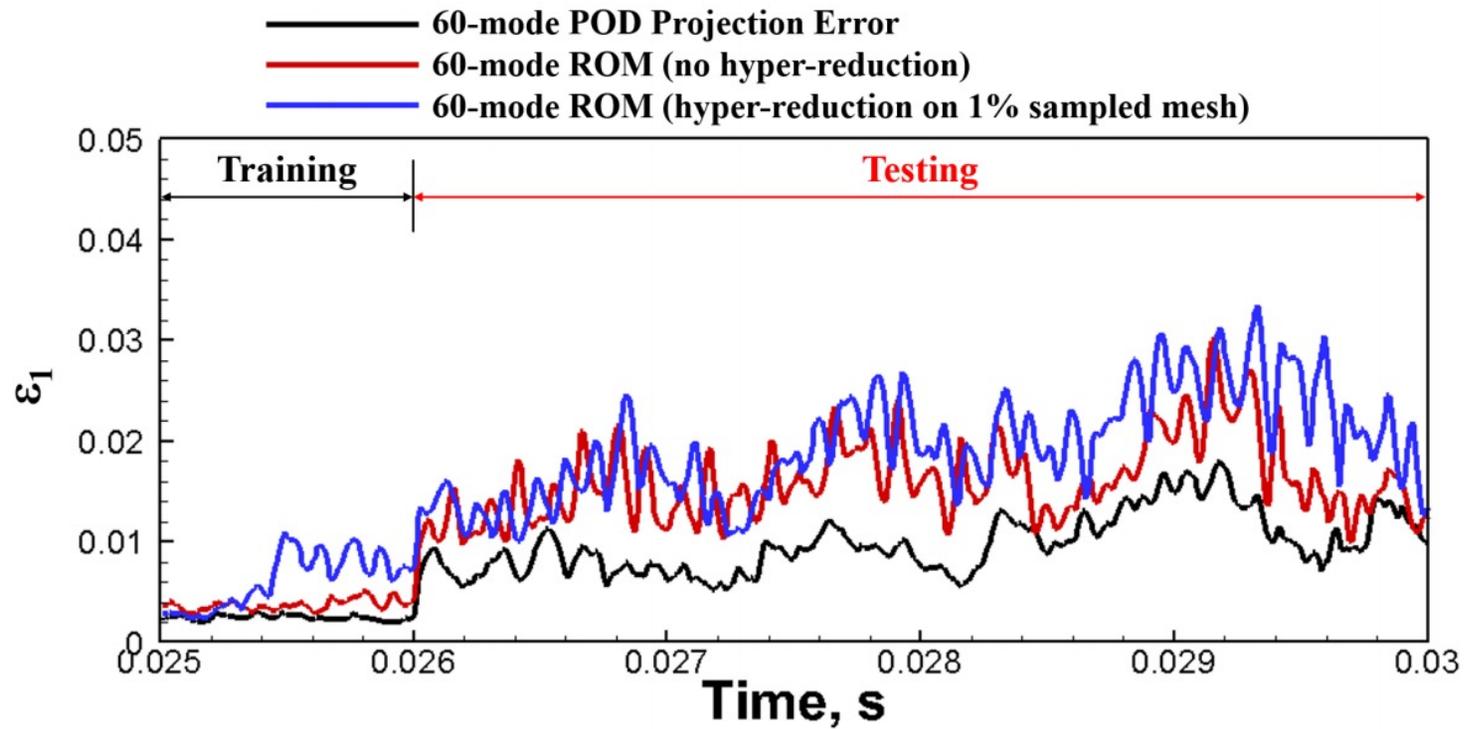


- Formulation
- Results

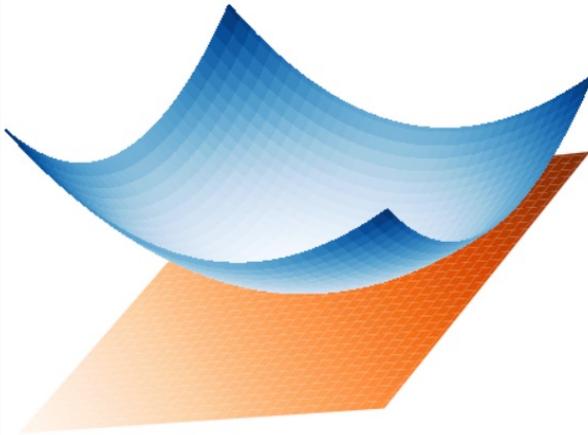
- Formulation
- Results

- Formulation
- Results

## Impact of projection error and sampling



$$d_n(\mathcal{A}, \mathcal{X}) = \inf_{\mathcal{X}_n} \sup_{x \in \mathcal{A}} \inf_{y \in \mathcal{X}_n} \|x - y\|_x$$



## Non-linear Manifold SP-LSVT

- Dual-time formulation w/r/t primitive state

$$\Gamma(\mathbf{s}) \frac{\partial \mathbf{s}}{\partial \tau} + \frac{\partial \mathbf{q}(\mathbf{s})}{\partial \mathbf{t}} - \mathbf{f}(\mathbf{q}) = \mathbf{0}, \quad \Gamma = \frac{\partial \mathbf{q}}{\partial \mathbf{s}}$$

- Introduce similar affine representation of primitive state

$$\mathbf{s} \approx \tilde{\mathbf{s}} = \bar{\mathbf{s}} + \mathbf{S}\Psi(\mathbf{s}_r) ; \quad \Psi : \mathbb{R}^K \rightarrow \mathbb{R}^N$$

- 

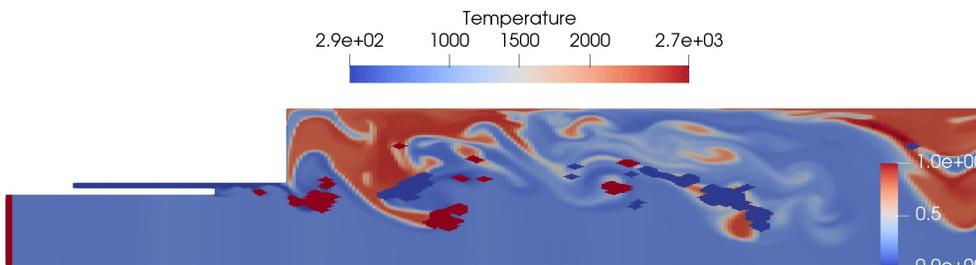
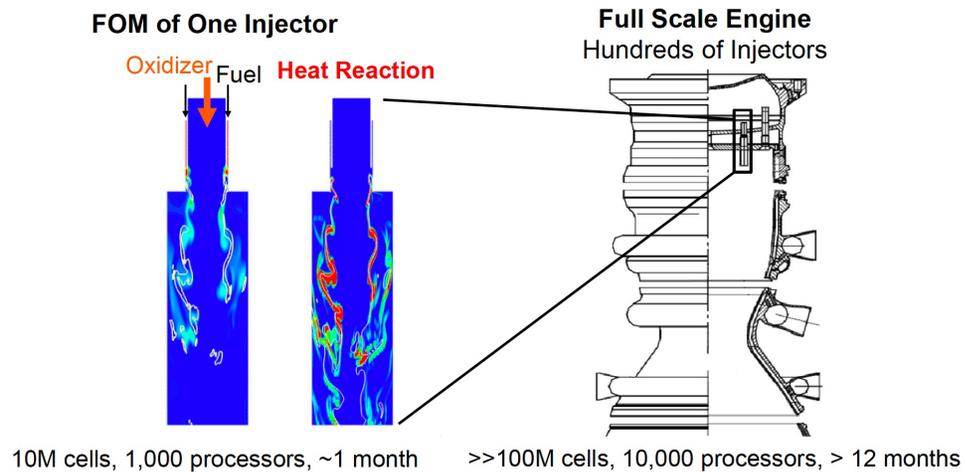
$$\mathbf{s}_r^n = \operatorname{argmin}_{\mathbf{a} \in \mathbb{R}^K} \|\mathbf{Q}\mathbf{r}_s(\bar{\mathbf{s}} + \mathbf{S}\Psi(\mathbf{a}))\|_2^2$$

$$(\mathbf{W}^{p-1})^T \mathbf{W}^{p-1} [\mathbf{s}_r^p - \mathbf{s}_r^{p-1}] = -(\mathbf{W}^{p-1})^T \mathbf{r}_s(\tilde{\mathbf{s}}^{p-1})$$

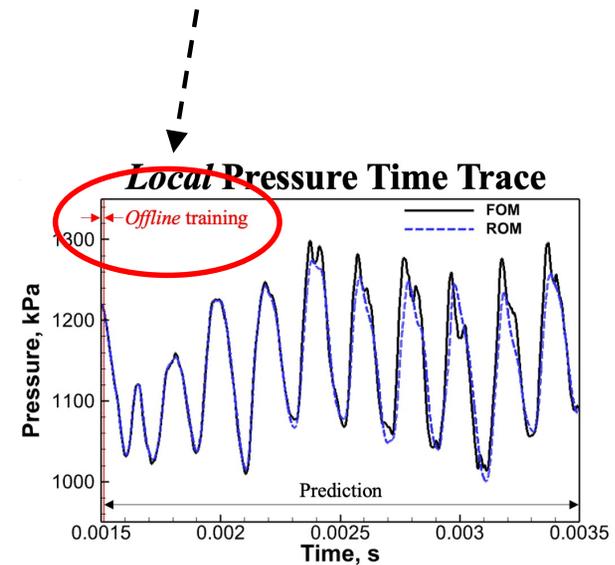
$$\mathbf{W}^{p-1} = \mathbf{Q} \frac{\partial \mathbf{r}_s(\tilde{\mathbf{s}}^{p-1})}{\partial \tilde{\mathbf{s}}} \mathbf{S} \left[ \frac{\partial \Psi}{\partial \mathbf{s}_r} \right]^{p-1}$$

- Symmetrized at sub-iteration level!
- Notice two levels of scaling:  $\mathbf{Q}$  and  $\mathbf{S}$

## Reducing computational complexity of extreme multi-scale problems while preserving mathematical and physical fidelity

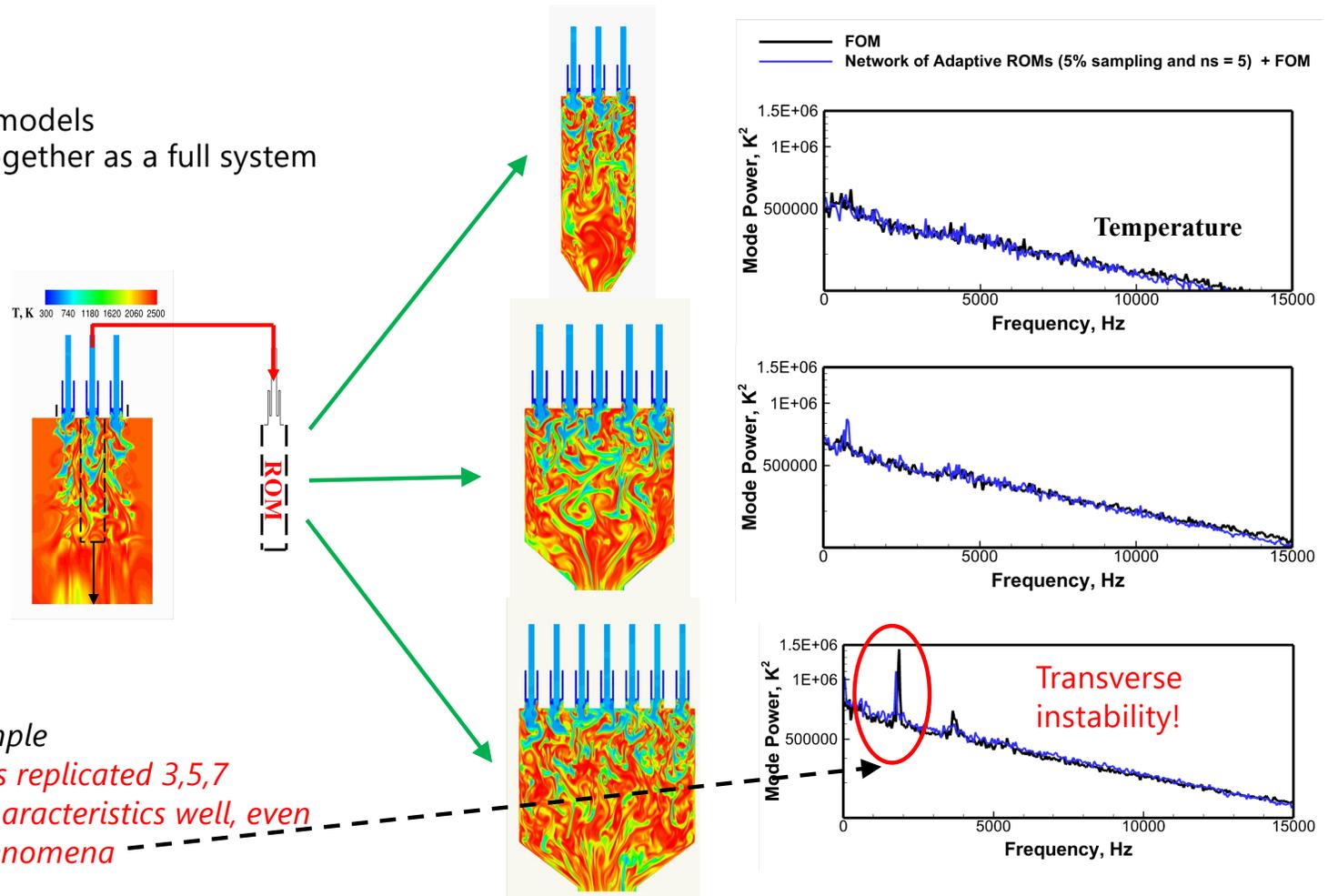


- In-situ adaptive sampling and projections to low-dimensional manifolds
- 2 orders of magnitude acceleration while preserving mathematical & physical fidelity
- **Future state and parametric prediction of extremely complex chaotic flows with negligible off-line training**



## Enabling reduced complexity modeling without having access to full system simulations

- Train component based models
- Integrate components together as a full system
- Execute adaptive ROMs



*Rocket combustor example*

*→ component ROM was replicated 3,5,7 times. It predicts flow characteristics well, even capturing emergent phenomena*