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Application of Reduced Order Modeling for Simulation of Turbulent Combustion

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Research Dialogues
April 15, 2020

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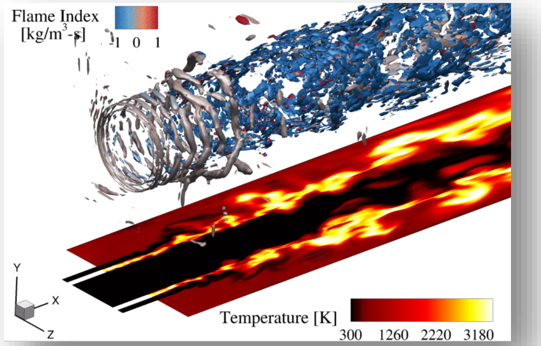
Outline

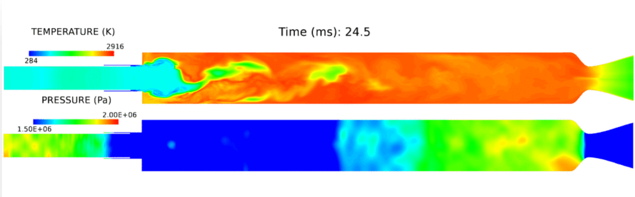
- Introduction
- Reduced Order Modeling Strategy
- Computational Setup
- Results
- Summary and Future Directions

Introduction

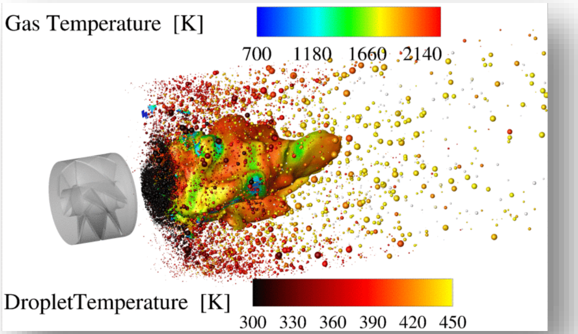
- Prediction of reacting flow physics in energy conversion and propulsion devices: challenging to experiments and simulations
- **Experimental challenges:** measurements limited to fewer quantities, expensive, etc.
- **Challenges to simulations:** uncertainties in geometry, boundary conditions, kinetics, closures, etc.
- **Large Eddy Simulation (LES)** is promising tool for prediction of reacting flow physics
- HPC advancements have allowed to perform high-fidelity LES, but computational expense still huge for design and optimization studies:
  - Grid resolution requirements
  - Tedious nonlinear calculation of thermodynamics, transport and chemical kinetics
  - Complex geometries



Stable Rocket Combustion[1]



Unstable Rocket Combustion[2]



Spray Combustion[3]

[1] *Ranjan et al., AIAA-2016-4999;* [2] *Srinivasan et al., FTC (2015);* [3] *Ranjan et al., AIAA-2016-4895*

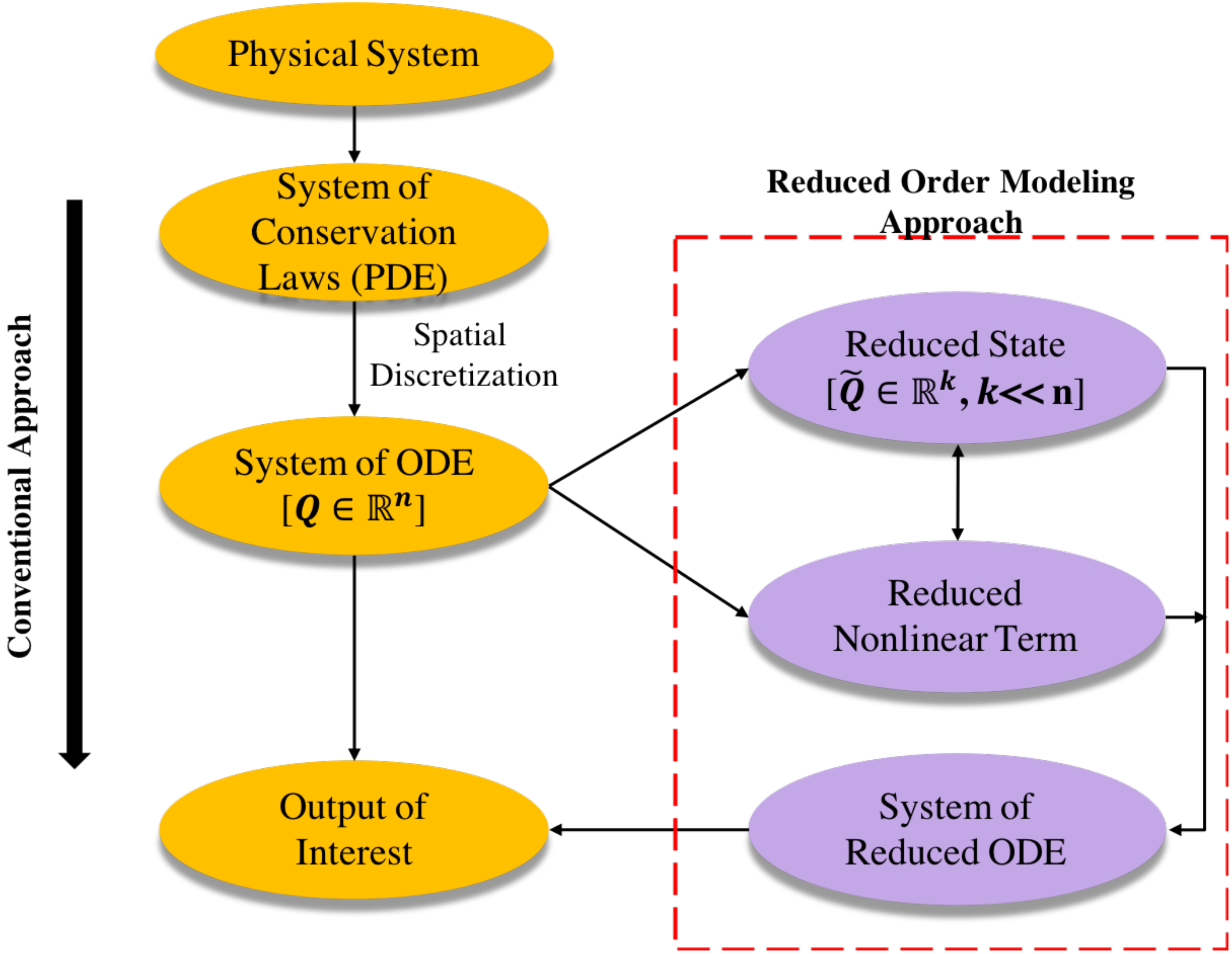
Introduction

- Typical cost of high-fidelity LES of practical devices: **about $\boldsymbol{O(10^5 - 10^6)}$ CPU hours**
- Parametric design studies under wide range of operating conditions to assess performance of propulsion device is computationally prohibitive
- High-fidelity reduced-order modeling (ROM): **a viable alternative**
- Several techniques to perform ROM of turbulent reacting flows: missing point estimation[1], linearization of governing system and weighted combination[2], empirical interpolation method[3], etc.
- Reduced Basis Modeling (RBM) is one of the ROM strategies, which can be used to perform computationally affordable high-fidelity simulations
- Preliminary investigation using ROM for LES showed promising results, but challenges also observed[4]
- **Objectives:**
  - Demonstrate features of two RBM based ROM strategies on a canonical setup
  - Assess accuracy and stability aspects of ROM strategies
  - Assess computational requirements for LES studies

[1] Astrid et al., IEEE Trans. Auto Control (2008); [2] Rewienski & White, IEEE Trans. CDICS (2003); [3] Grepl et al., ESAIM (2007); [4] Ranjan et al., AIAA-2018-4871

Reduced Order Modeling Strategy

Conventional vs ROM Enabled CFD



Physical System

System of Conservation Laws (PDE)

Spatial Discretization

System of ODE $[\boldsymbol{Q} \in \mathbb{R}^{n}]$

Output of Interest

Conventional Approach

Reduced Order Modeling Approach

Reduced State $[\tilde{\boldsymbol{Q}} \in \mathbb{R}^{k}, \boldsymbol{k} << \mathbf{n}]$

Reduced Nonlinear Term

System of Reduced ODE

Mathematical Formulation

Semi-discrete PDE $$\frac{d\boldsymbol{q}(\boldsymbol{x},t)}{dt} = \boldsymbol{A}\boldsymbol{q} + \tilde{\boldsymbol{f}}(\boldsymbol{x},t)$$

Reduced-order representation of state vector $$\boldsymbol{q}(\boldsymbol{x},t) \approx \boldsymbol{Q}(\boldsymbol{x})\tilde{\boldsymbol{q}}(\boldsymbol{t})$$

$\boldsymbol{q}$: Composite state vector
$\boldsymbol{A}$: Linear dynamics
$\tilde{\boldsymbol{f}}$: Nonlinear terms
$\boldsymbol{Q}(\boldsymbol{x})$: Space-dependent POD based basis functions of $\boldsymbol{q}(\boldsymbol{x},t)$

POD[1] based ROM

$$\frac{d\tilde{\boldsymbol{q}}}{dt} = \boldsymbol{Q}^T\boldsymbol{A}\boldsymbol{Q}\tilde{\boldsymbol{q}} + \boldsymbol{Q}^T\tilde{\boldsymbol{f}}(\boldsymbol{Q}\tilde{\boldsymbol{q}})$$

- Suitable for linear problems
- Snapshots required for only state vector
- No gain in efficiency for non-linear problems

POD-DEIM[2] based ROM

$$\frac{d\tilde{\boldsymbol{q}}}{dt} = \boldsymbol{Q}^T\boldsymbol{A}\boldsymbol{Q}\tilde{\boldsymbol{q}} + (\boldsymbol{Q}^T\boldsymbol{U})(\boldsymbol{P}^T\boldsymbol{U})^{-1}\tilde{\boldsymbol{f}}(\boldsymbol{P}^T\boldsymbol{Q}\tilde{\boldsymbol{q}})$$

- Suitable for non-linear problems
- Snapshots required for state vector, fluxes and source terms
- Significant gain for non-linear problems

$$\boldsymbol{q} \in \mathbb{R}^{r\times 1}, \tilde{\boldsymbol{f}} \in \mathbb{R}^{r\times 1}, \boldsymbol{A} \in \mathbb{R}^{r\times r}$$
$$\boldsymbol{q} = [\rho, \rho\boldsymbol{u}, \rho\boldsymbol{v}, \rho\boldsymbol{w}, \rho E, \rho k^{sgs} \rho Y_1, \rho Y_2, \dots, \rho Y_s]^T$$

$$\boldsymbol{Q} \in \mathbb{R}^{r\times k}, \tilde{\boldsymbol{q}} \in \mathbb{R}^{k\times 1},$$
$$\boldsymbol{U} \in \mathbb{R}^{r\times k}, \boldsymbol{P} \in \mathbb{R}^{r\times n}$$

$$\boldsymbol{k} \ll \boldsymbol{r}, \qquad \boldsymbol{n} \ll \boldsymbol{r}$$

POD: Proper Orthogonal Decomposition
DEIM: Discrete Empirical Interpolation Method

[1] *Wilcox & Peraire, AIAA J., 40 (2002)*
[2] *Chaturantabut & Sorensen, SIAM J. Sci., 32 (2010)*

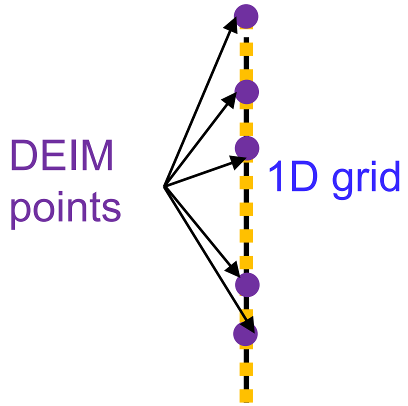
POD and POD-DEIM based ROM

- Consider the linear 1D advection equation:

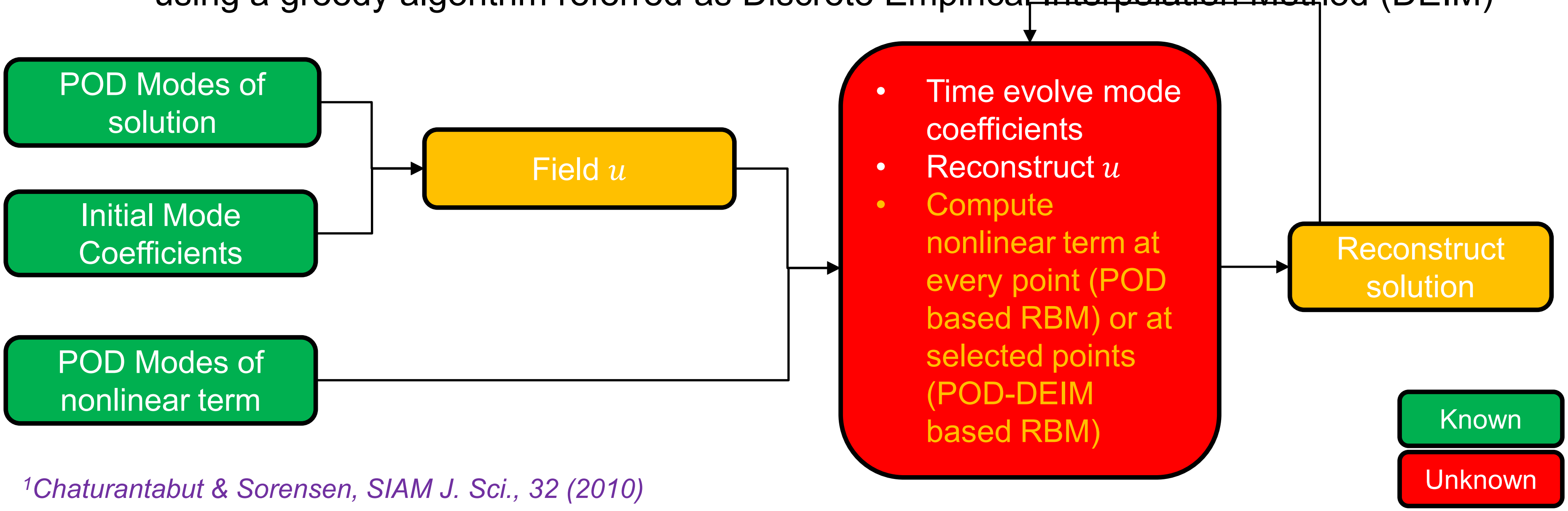
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$$

- POD based RBM: $\mathrm{u} \approx \phi(x)\tilde{u}(t)$

$$\phi\frac{d\tilde{u}}{dt} = -([\boldsymbol{\phi}][\tilde{\mathbf{u}}])\left(\left[\frac{d\boldsymbol{\phi}}{dx}\right][\tilde{\mathbf{u}}]\right) \approx N(u)$$



- POD-DEIM based RBM:
  - **Approximates nonlinear term**
  - Evaluates nonlinear term only at certain points in the domain, which are determined using a greedy algorithm referred as Discrete Empirical Interpolation Method (DEIM)[1]



POD Modes of solution

Initial Mode Coefficients

POD Modes of nonlinear term

Field u

- Time evolve mode coefficients
- Reconstruct u
- Compute nonlinear term at every point (POD based RBM) or at selected points (POD-DEIM based RBM)

Reconstruct solution

🟩 Known

🟥 Unknown

[1] *Chaturantabut & Sorensen, SIAM J. Sci., 32 (2010)*

ROM Enabled CFD Solver

- ROM based approaches implemented within LESLIE[1]
- LESLIE is a fully compressible, multi-species Navier-Stokes solver[2]
- **Three stage solution strategy:**
  - Stage 1: assembly of snapshots
  - Stage 2: extraction of POD modes and selection of DEIM points
  - Stage 3: computation of ROM solution
- **Implementation details:**
  - All stages are memory intensive compared to a baseline CFD solver: **challenging for 3D and complex applications**
  - Stage 1 and 3 are fully parallel: use parallel decomposition
  - Stage 2 is serial
- **Key Challenges:**
  - Memory requirements and complex data-structure
  - Offline analysis is tedious: parallelization may help or other approaches can be considered to reduce memory footprint

[1] *Ranjan et al., AIAA-2018-4871*; [2] *Genin & Menon, AIAA J. (2010)*

Example:1D Complex Ginzburg-Landau Equation

- Complex Ginzburg-Landau equation (GLE):

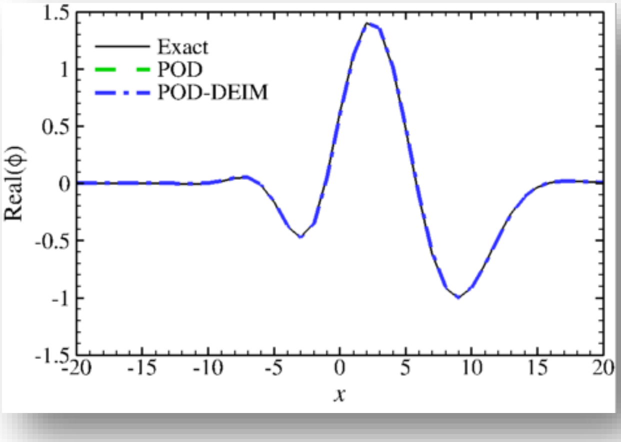
$$\frac{\partial \phi}{\partial t} + \nu \frac{\partial \phi}{\partial x} = \gamma \frac{\partial^2 \phi}{\partial x^2} + \mu \phi - a|\phi|^2 \phi$$

$$x \in [-50,50]$$

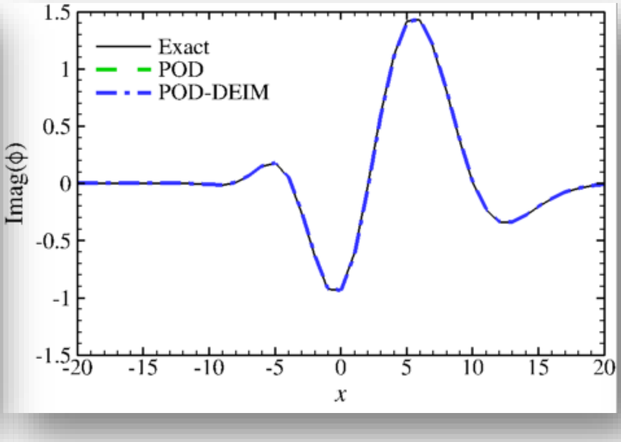
$$\phi(x = -50, t) = 0, \frac{\partial \phi}{\partial x}\bigg|_{x=50} = 0$$

- Coefficients ν and γ are complex leading to complex solution
- Time evolution of solution at a specified location shows a limit cycle behavior
- Simulation details:
  - Number of points = 101
  - **Number of snapshots = 251**
  - Number of POD modes = 6
  - Number of DEIM points = 6
- Results compared at final time T = 200 units

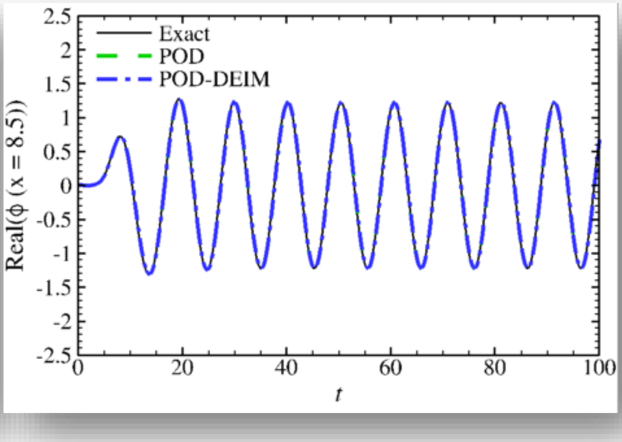
Example: Comparison of Final Solution



Real part of solution at T = 200 units



Imaginary part of solution at T = 200 units



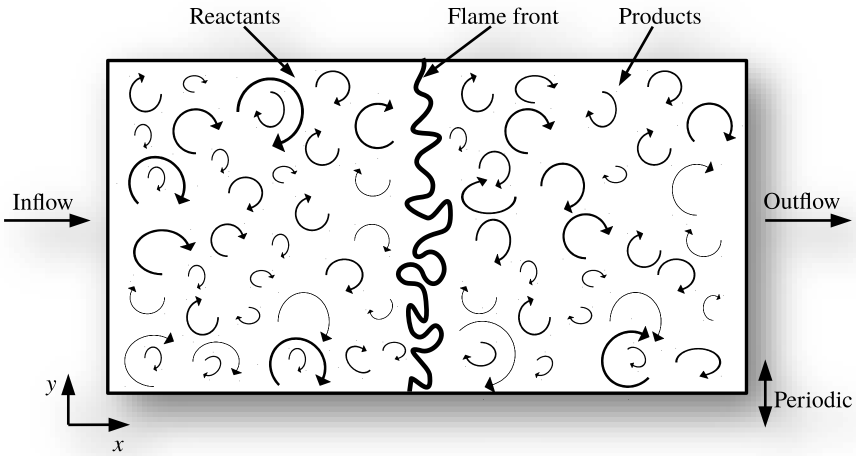
Time evolution of real part of solution at x = 8.5

- Solutions with POD (**6 modes**) and POD-DEIM (**6 modes and 6 DEIM points**) methods show excellent agreement with exact solution at T = 200 units
- Solution exhibit a limit cycle behavior over a long period of time
- **Comparison of cost:**
  - Exact: 32.5 s, POD: 19.9 s, POD-DEIM: 2.5 s
  - Cost reduces by around 16 times with POD-DEIM approach
- **Although fewer number of modes yield accurate results, but 251 snapshots were used during analysis stage**

Computational Setup

3D Turbulent Premixed Flame

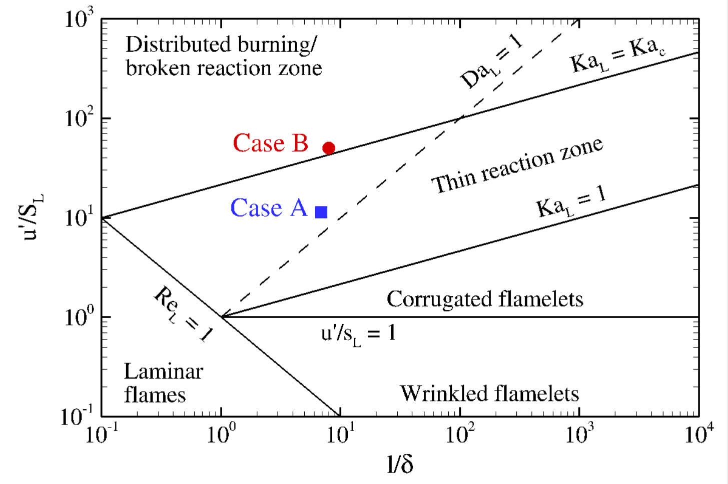
- LES of freely propagating methane/air turbulent premixed flame
- Flame Conditions[1,2]: $\phi = 0.8, \mathrm{T_{ref}} = 300\ \mathrm{K}, \mathrm{P_{ref}} = 1\ \mathrm{atm}$
- Finite-rate kinetics effects employed using a 4-step and 8-species mechanism[3]
- 3D domain with characteristic based inflow/outflow boundary conditions and periodic conditions in transverse and spanwise directions
- Initialization based on laminar solution imposed on background turbulent flow



Schematic of computational domain

Case	$N_x \times N_y \times N_z$	u'/S_L	l/δ
A	96^3	10	6.2
B	128^3	50	9.6

Simulation Parameters



Premixed flame regime diagram

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[1] Ranjan et al., CST (2016); [2] Panchal et al., CST (2019); [3] Peters (2000)

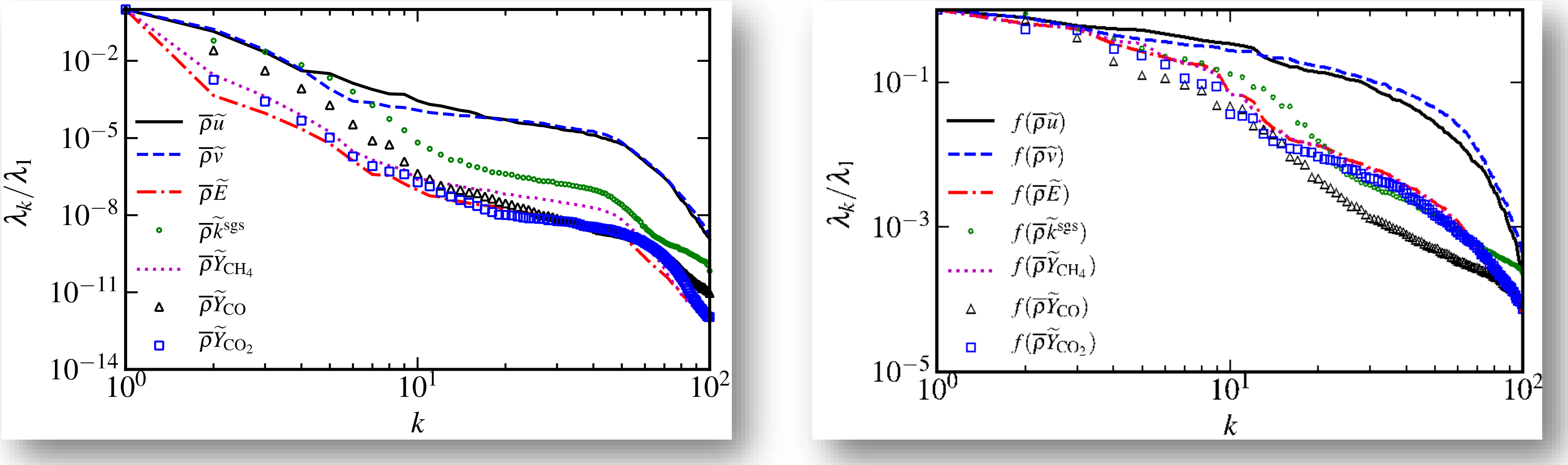
Numerical Methodology

- Baseline simulations are performed using LESLIE[1]:
    - Block structured finite-volume solver
    - Spatial discretization: hybrid scheme blending 2nd order MacCormack
    - Time integration: 2nd order explicit
    - Characteristics based boundary conditions
    - Power law transport with thermally perfect gas assumption for EoS
- Subgrid-scale (SGS) closures:
    - Momentum and energy flux: eddy viscosity based on the SGS turbulent kinetic energy[2]
    - Turbulent combustion: quasi-laminar chemistry (QL[3])
- ROM based LES for each case:
    - 100 snapshots saved from baseline simulation for 1 eddy turnover time
    - POD and POD-DEIM based ROM performed using different number of modes and DEIM points

[1]Genin & Menon, AIAA J. (2010); [2]Kim & Menon, (1999); [3]Grinstein & Kailasanath, CF (1995)

Results

Modal Analysis: Eigenvalues



State Vector

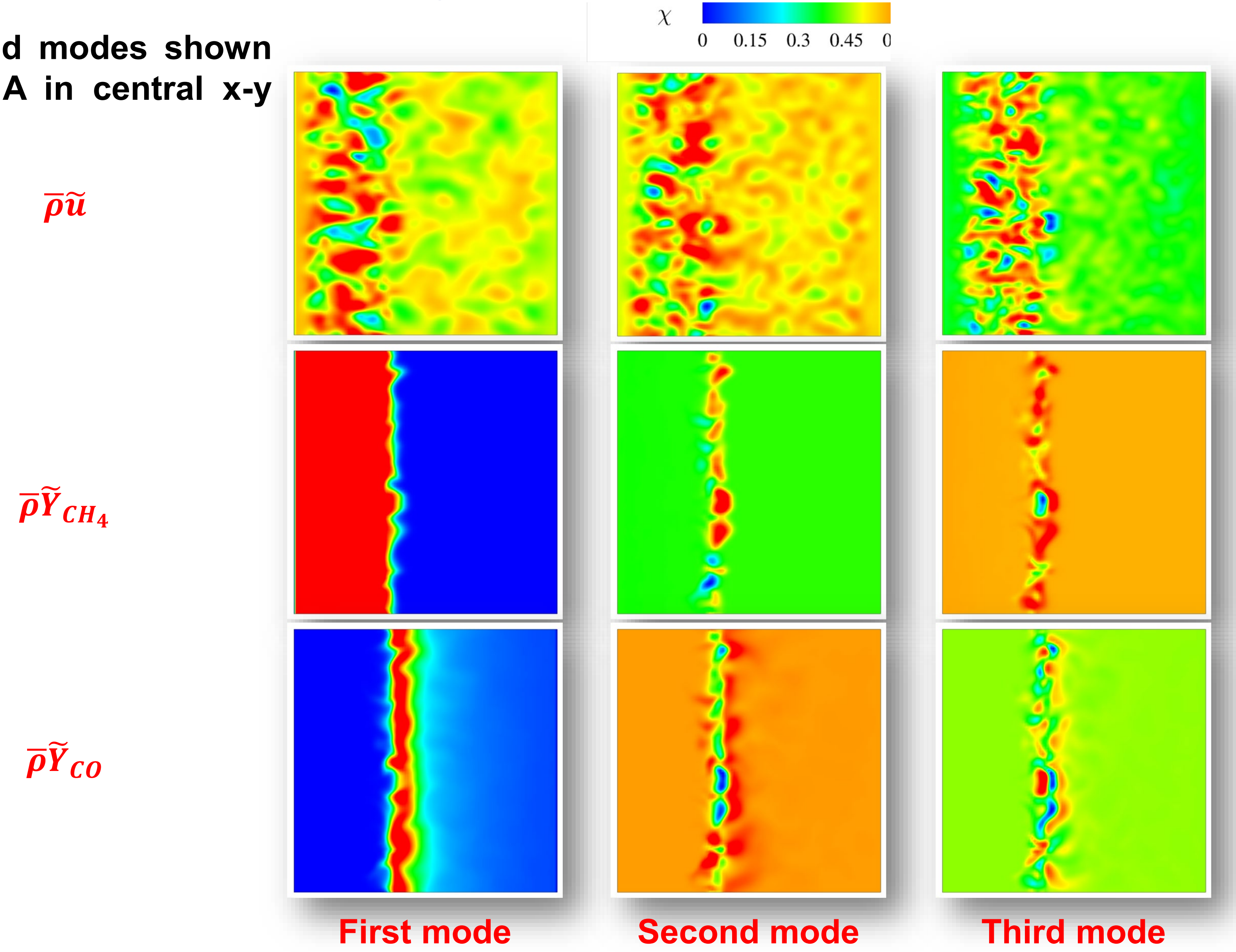
Nonlinear terms

Normalized eigenvalues for Case A

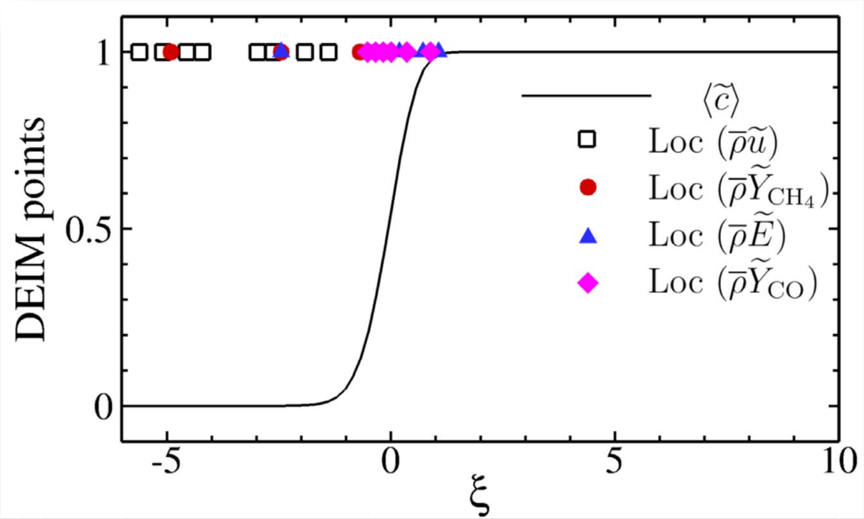
- Normalized eigenvalues shown for some components of state vector and nonlinear term: **behavior is same in case B**
- Eigenvalues decay with increase in mode index: **ROM can be performed**
- Rate of decay differs for different variables and for nonlinear terms
- Overall 10 modes seem to be adequate

Modal Analysis: Spatial Behavior

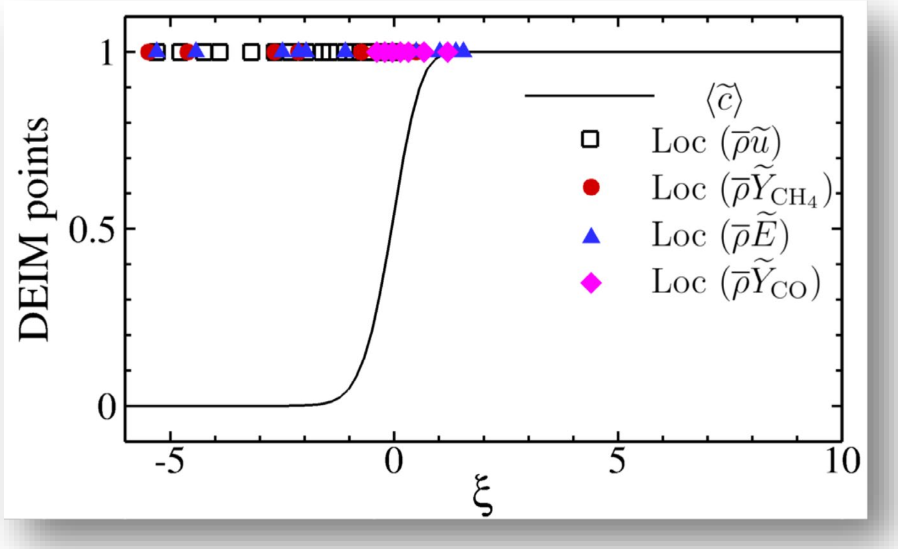
Normalized modes shown for Case A in central x-y plane



Analysis using DEIM (Case A)



Number of POD modes: 10
Number of DEIM points: 10

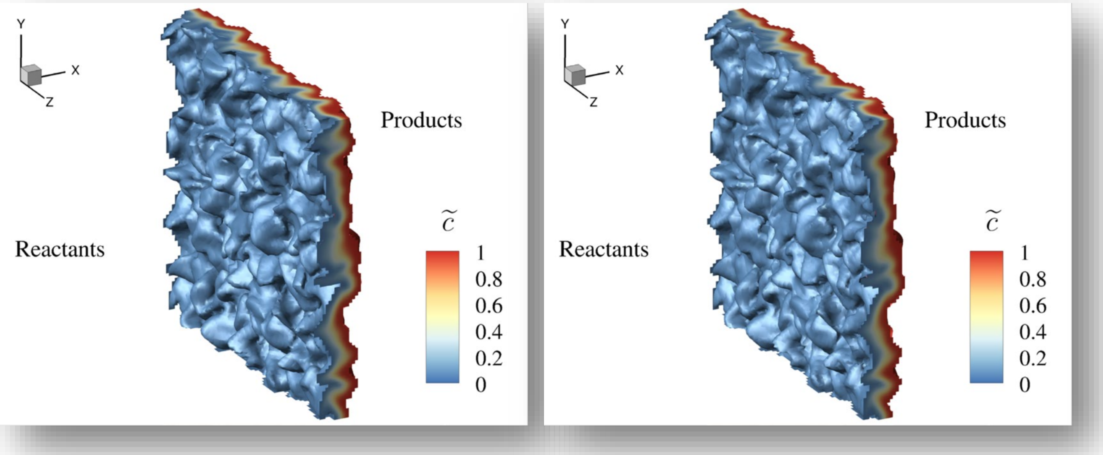


Number of POD modes: 10
Number of DEIM points: 20

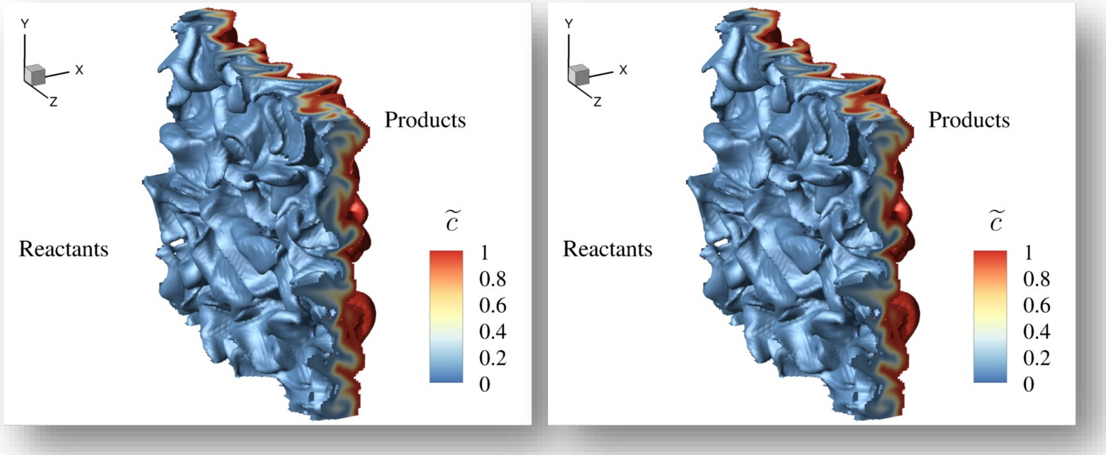
- Location of points identified by DEIM across the flame brushes for representative variables
- Points are concentrated in preheat region and regions of heat release
- Points for thermo-chemical quantities correspond to region of heat release as these quantities vary significantly in such regions
- DEIM appropriately responds to underlying dynamics of this problem

Structural Features of Flame Brush

- Structure of flame brush captured very well by POD based ROM compared to baseline cases after 1 eddy turnover time
- Disruption of initially planar flame by turbulent eddies
- Continuous reaction zone as expected for flames in TRZ regime
- Increase in length scales in post-flame region due to thermal expansion



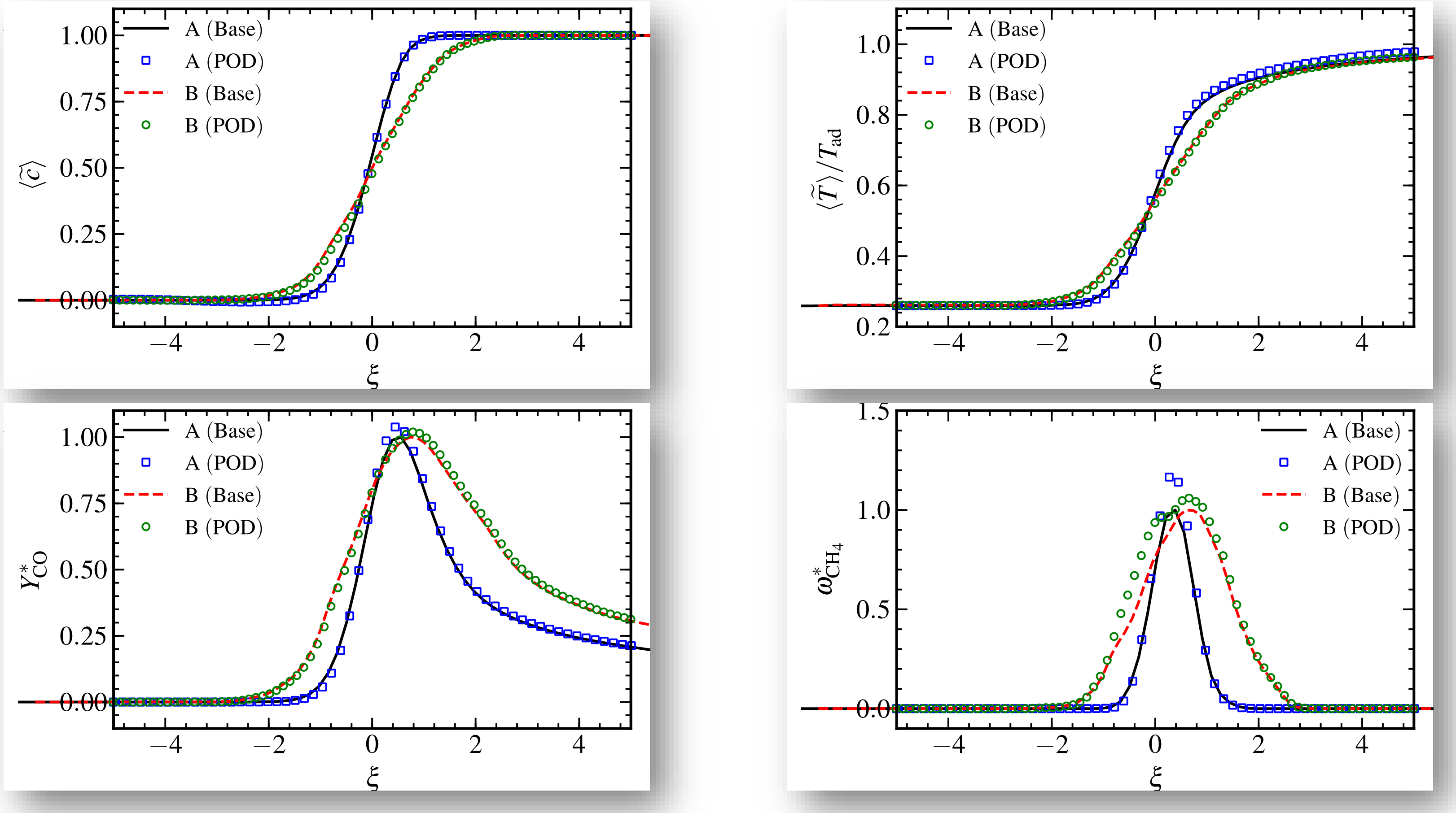
Case A



Case B

Baseline **POD based ROM**

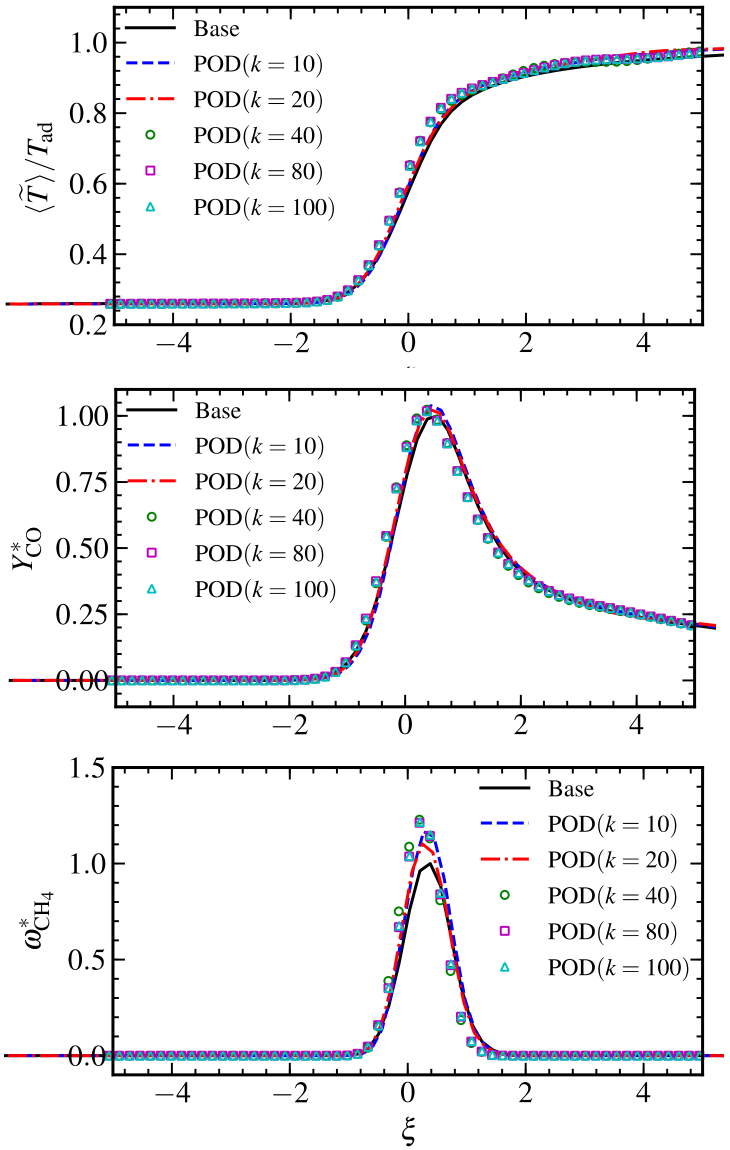
Spatially Averaged Flame Structure



- Comparison of spatially averaged flame structure obtained using POD based ROM cases (10 modes) with baseline cases after $t/t_0 = 1$
- Good agreement observed where effect of increase in turbulence level captured by POD based ROM

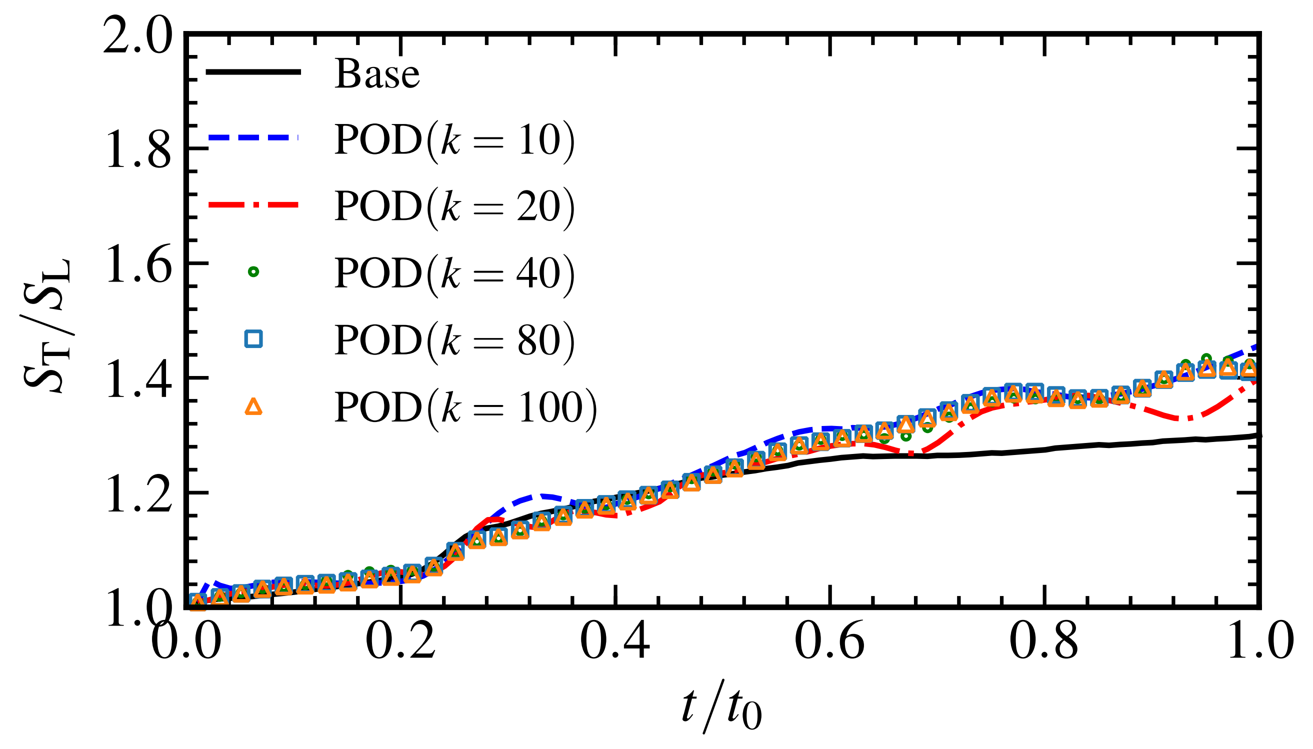
Spatially Averaged Flame Structure (Case A)

- Comparison of spatially averaged flame structure obtained using POD based ROM cases with baseline cases after $t/t_0 = 1$
- Effect of increase in number of POD modes from k = 10 to k =100 shows no significant improvements in results
- Overall, 10-20 modes tend to be reasonable
- Profiles of outputs of interest show excellent agreement, but differences are observed in profiles of reaction rate
- Till $t/t_0 = 0.5$, even reaction rate profiles yield excellent agreement (not shown here)



Results from Case A at $t/t_0 = 1$

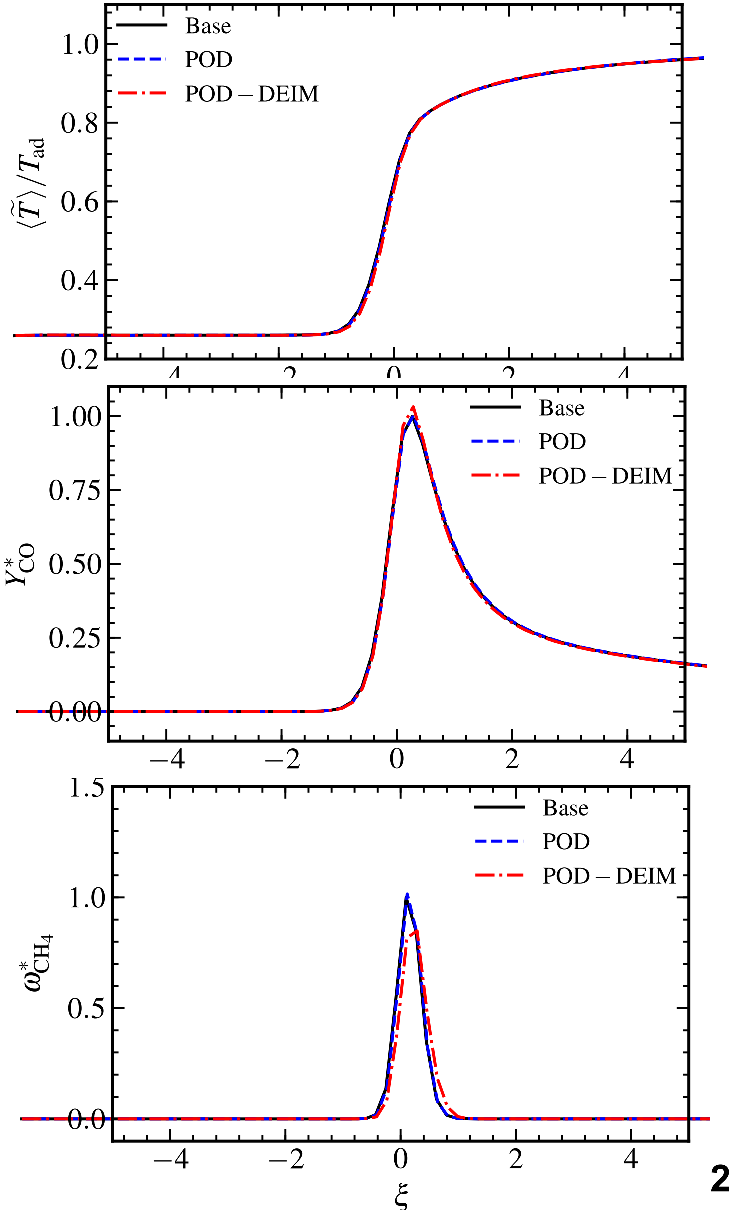
Time Evolution of Turbulent Flame Speed (Case A)



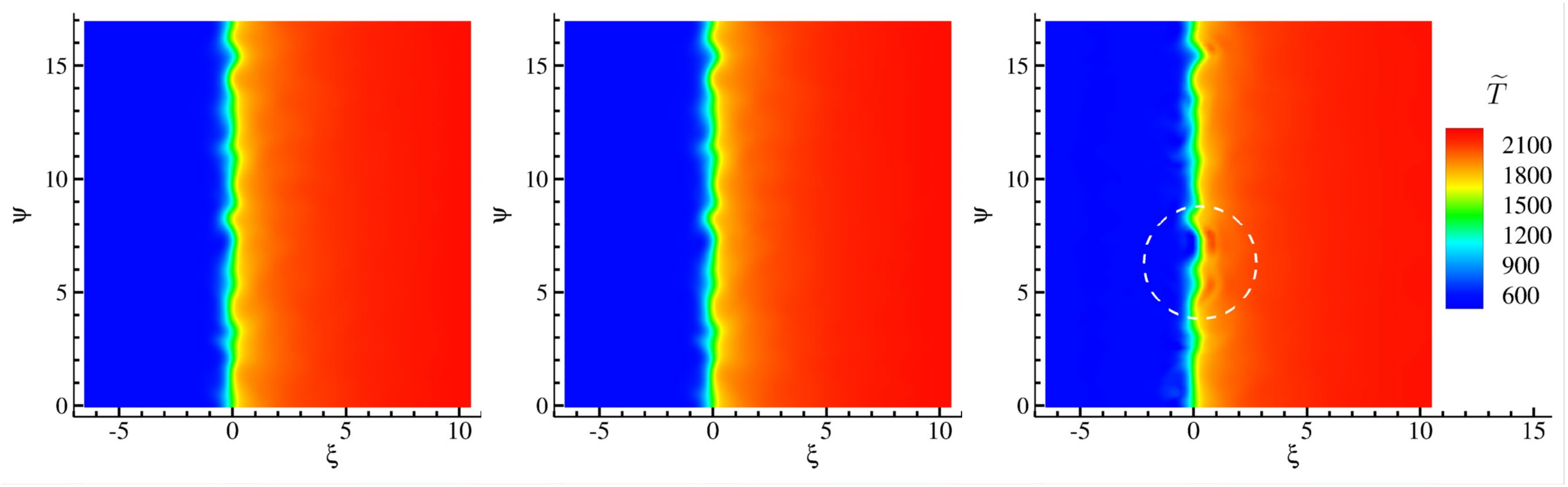
- Evolution of normalized turbulent flame speed used as a global metric to assess accuracy of results from Case A
- A maximum differences by about 8% occurs at final time
- Again, 10-20 modes can be considered adequate

Baseline, POD and POD-DEIM (Case A)

- POD-DEIM based ROM observations:
    - 10 POD modes considered
    - Numerical instability observed beyond $t/t_0 = 0.5$ irrespective of number of DEIM points
    - Results compared for case with 10 POD modes and 10 DEIM points at $t/t_0 = 0.2$
- Profile of temperature show excellent agreement with baseline and POD results
- Intermediate species show a minor over-prediction in peak values
- Reaction rate of fuel is underpredicted: only at 10 points evaluation of reaction rate performed with POD-DEIM based ROM
- Instability tend to be associated with thermodynamics



Instability with POD-DEIM based ROM (Case A)



Baseline **POD** **POD-DEIM**

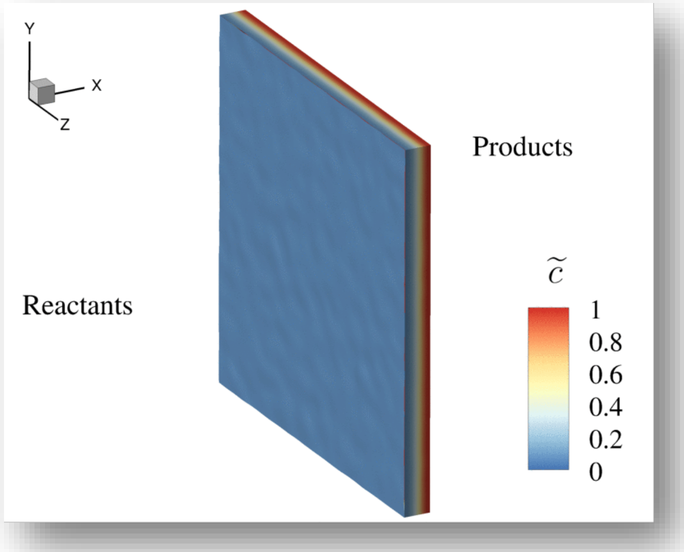
- Contours of temperature shown in central plane at $t/t_0 = 0.24$ for Case A
- Abrupt increase and decrease in temperature occurs in POD-DEIM near flame region
- Further analysis underway (results from these studies will be included):
  - Increase in DEIM points do not improve results
  - Increase in POD modes for fixed number of DEIM points being evaluated
  - Evolution of extremum of pressure field underway

Summary and Future Directions

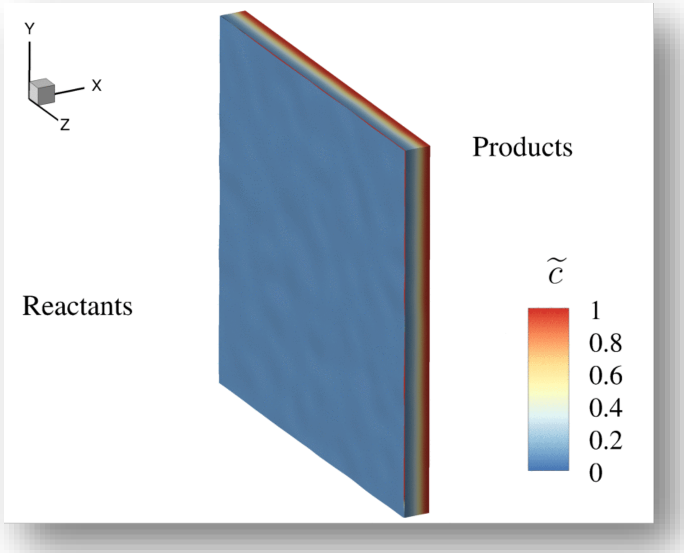
- Assessment of high-fidelity ROM approaches for LES of canonical chemically reacting turbulent flows
- Two ROM strategies considered: POD and POD-DEIM
- Both approaches are implemented in a well-established multiphysics compressible flow solver
- POD based ROM yields good agreement with baseline results for flames interacting with different levels of turbulence
- POD-DEIM showed onset of spurious numerical oscillations after certain time leading to divergence of results
- **Further studies:**
    - Improve computational efficiency of offline analysis stage
    - Assess stability aspects of POD-DEIM in terms of role of thermodynamics
    - Reduce memory footprint to allow for efficient simulation of practical systems and simplify data-structure

Thank You

Questions?



Case A



Case B