Requirements Towards Predictive Simulations of Combustion in Rocket Motors

MATTHIAS IHME

WITH: WAI TONG CHUNG, HAO WU, AND NIKOLAS PERAKIS

Department of Mechanical Engineering
Stanford University

Challenges in Predicting Turbulent Combustion

Need
- Emission:
- CO, NOx, soot, etc.
- Dynamics:
- stabilization, thermo-acoustic instabilities

Opportunities
- Computational resources
- Optimization and control
- Complex combustion modes, operating conditions, fuels

Challenge
- Complex flame topology
- Scale separation and physical coupling
- Chemical complexity
- Stiff chemical reactions

Requirements
- Accuracy and error control
- Computational efficiency and scalability
- Engineering application

What is the purpose of a combustion simulations?

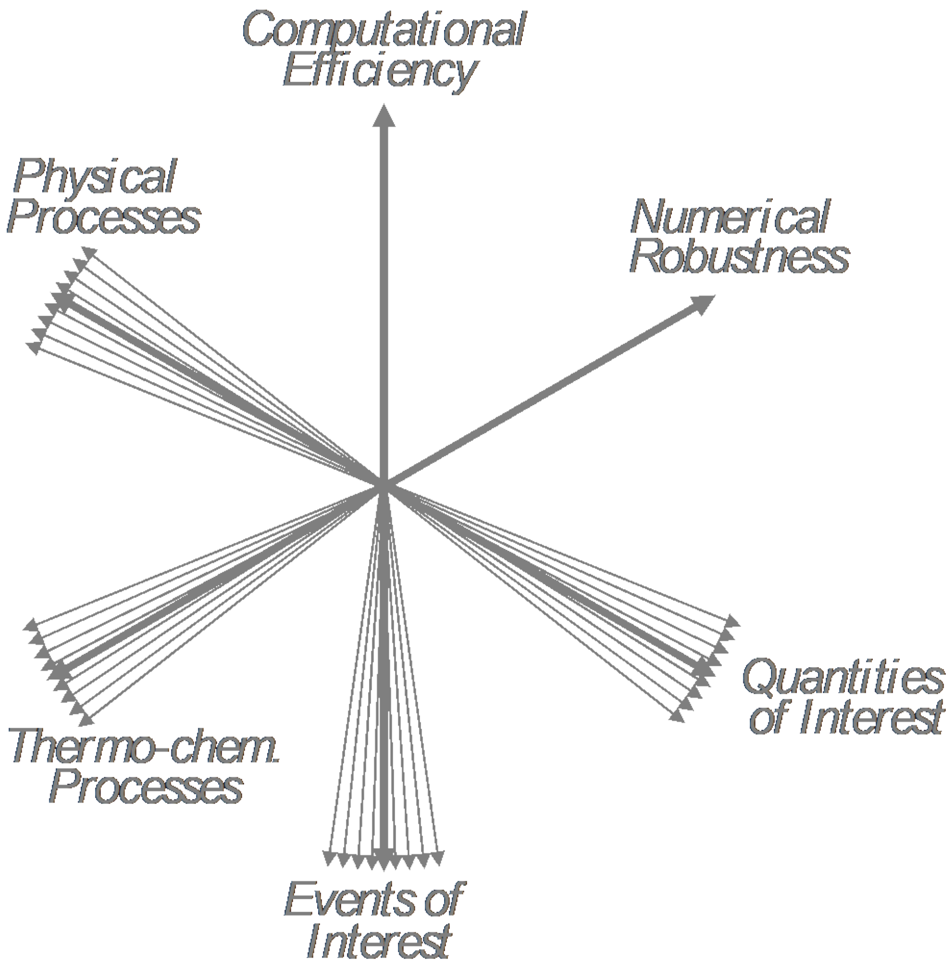
How should a combustion model be selected?

What is the impact of the numerical discretization on the combustion simulation?

How to assess the simulation accuracy?

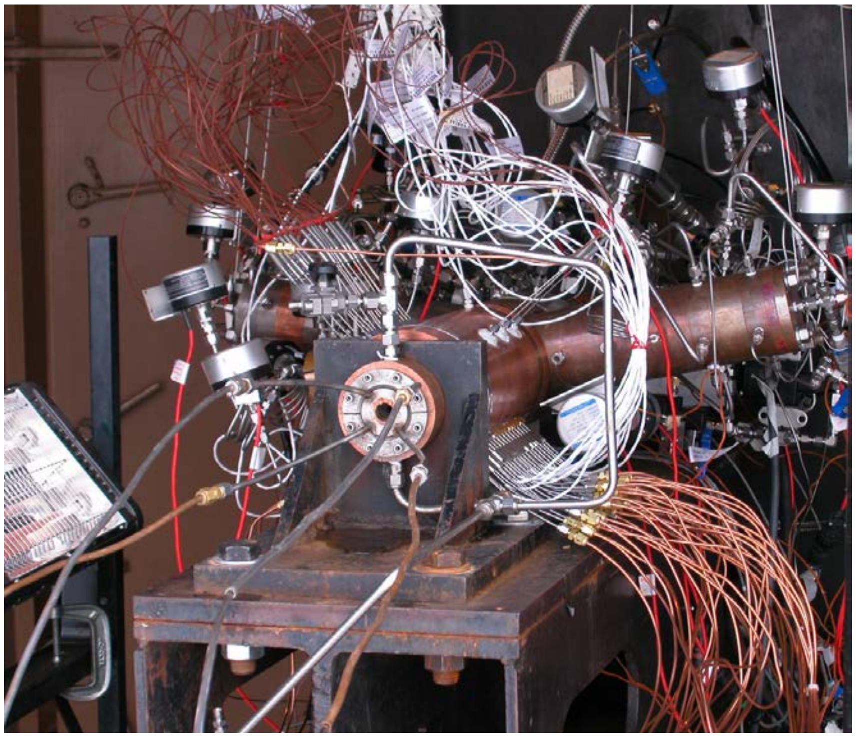
How can simulations be augmented with experimental data?

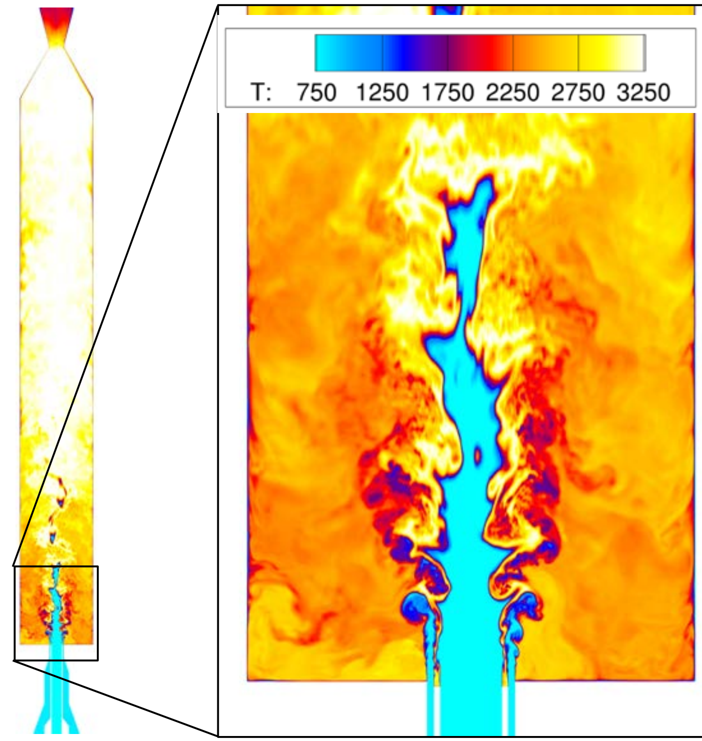
Model Performance



Combustion Modeling Approaches

RCM1 Injector: Complex Multi-Mode Combustion Modes





Combustion Modeling Approaches

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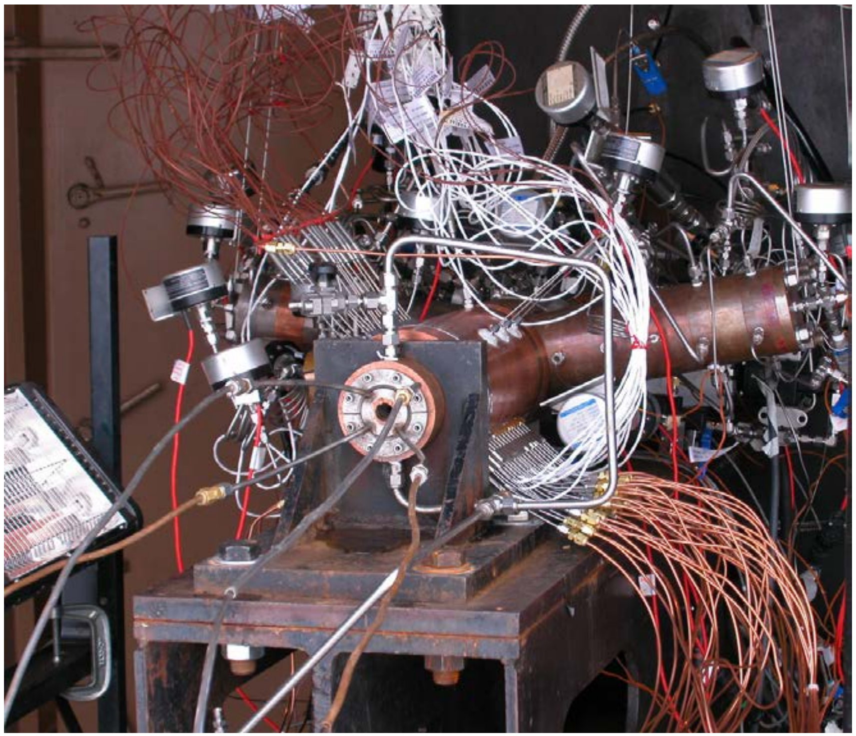
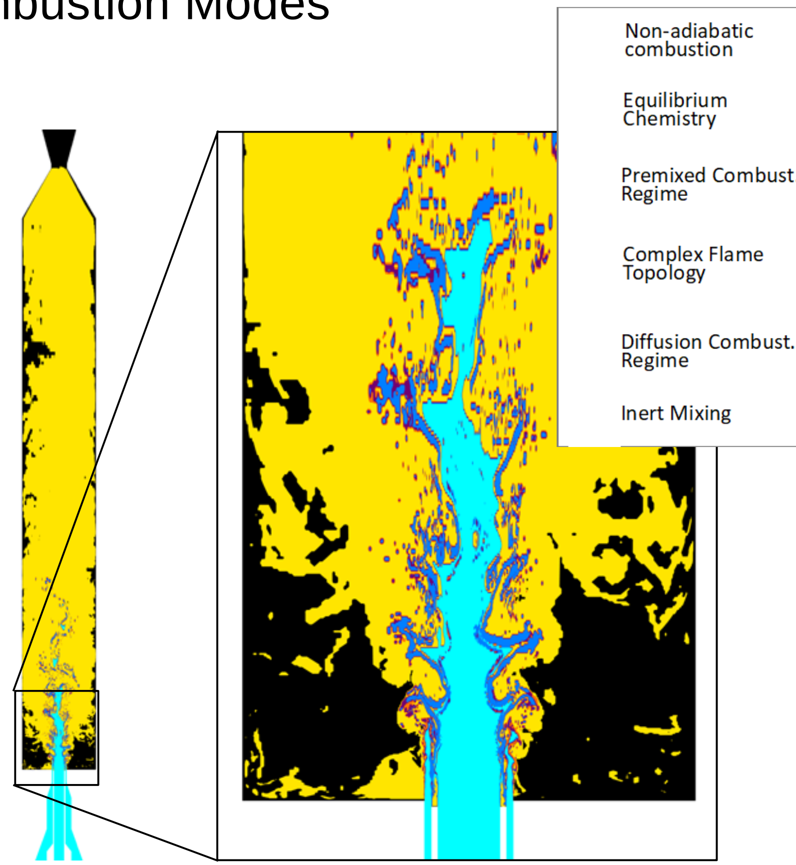




Combustion Modeling Approaches

Topology-based combustion models

- Construct from canonical flame configurations

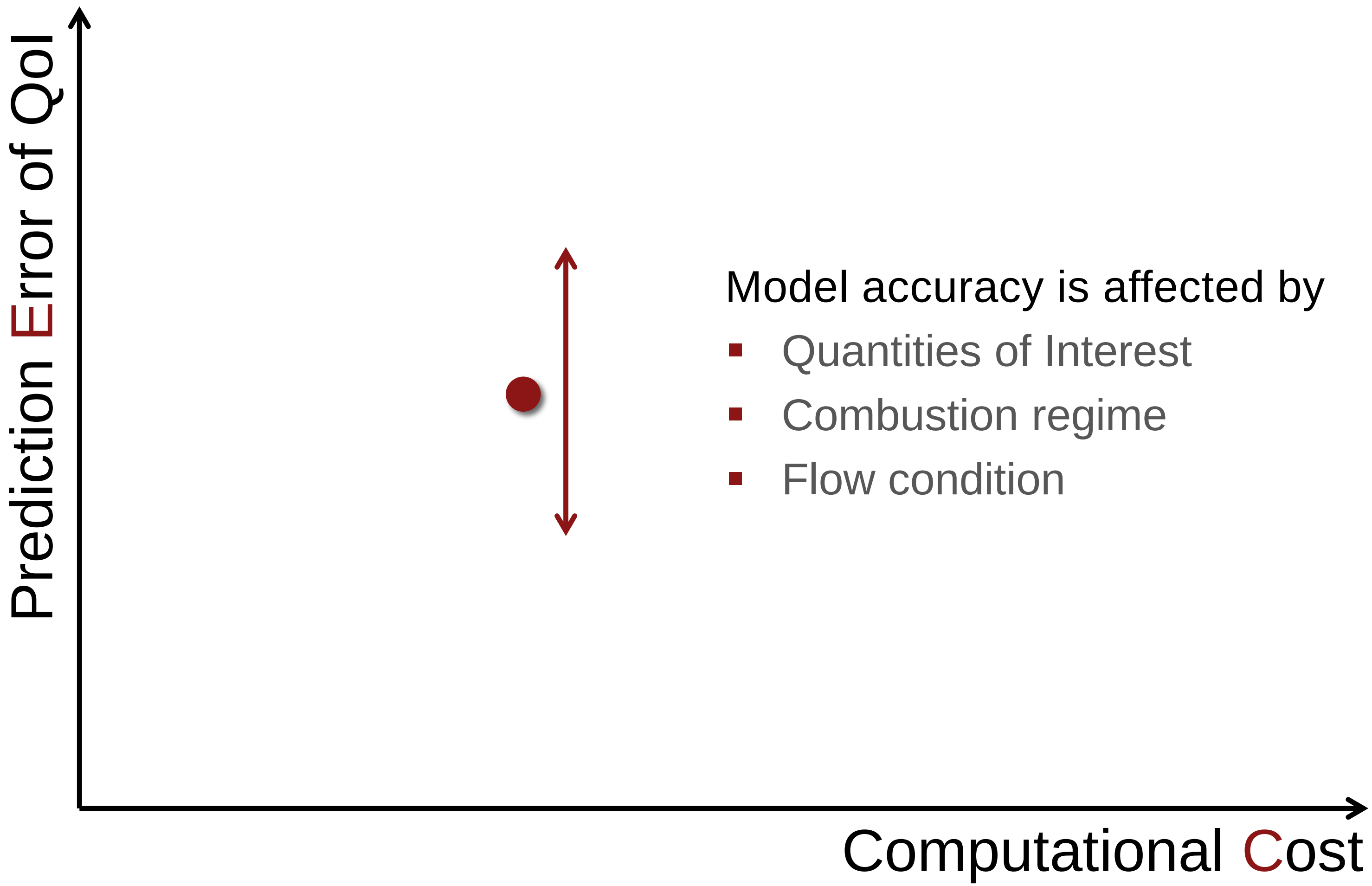
FPI, FGM, etc.)

Topology-free combustion models

- Detailed/reduced chemical mechanism
- High manifold dimensionality (20-40)
- Examples: DRG, PFA, QSS, PE, RCCE

How to select the "right" combustion models?

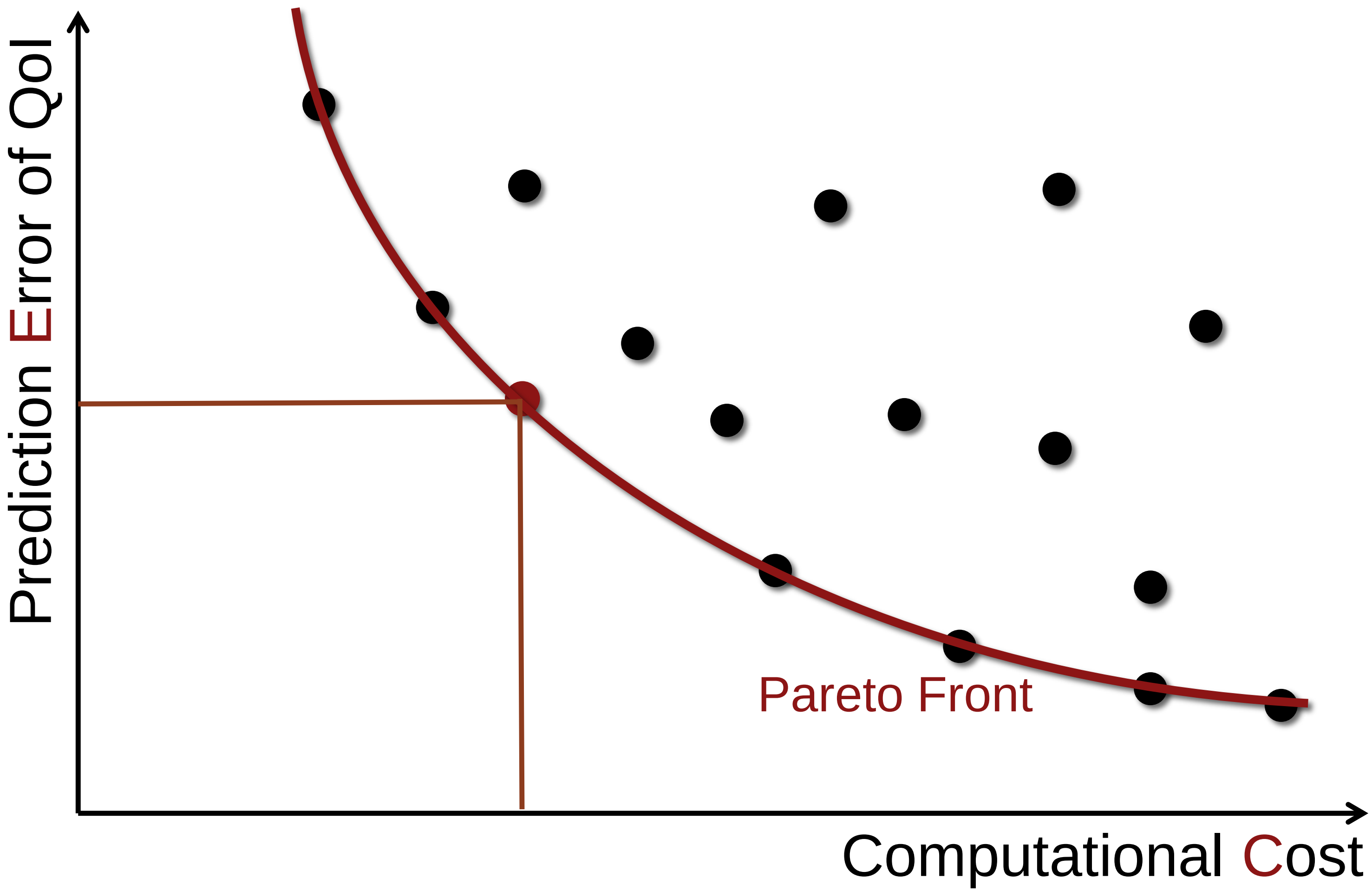
Performance of Combustion Models



Model accuracy is affected by

- Quantities of Interest
- Combustion regime
- Flow condition

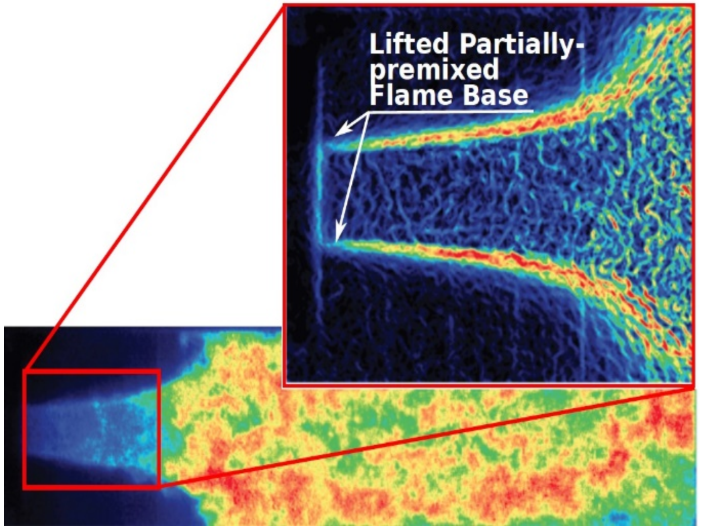
Performance of Combustion Models



Performance of Combustion Models

Issues with model-selection

- Model error depends on
  - Quantities of interest (T, CO2, CO, NO)
  - Combustion-physical processes (autoignition, local extinction/re-ignition)
  - Combustion regimes: premixed, non-premixed, multiphase



Lifted and partially-premixed flame base in LOX/GCH4 supercritical combustion

Objective

- Develop Pareto-efficient combustion (PEC) framework for optimal submodel assignment, under consideration of user-specific input about
  - Quantities of interest
  - Set of combustion submodels
  - Desired accuracy and cost

PEC Modeling Framework

User input

- Set of quantities of interest: $Q = \{Y_{CO2}, Y_{CO}, Y_{H2O}, Y_{NO}, \ldots\}$
- Set of candidate combustion models: M
  - Reaction-transport manifolds: FPV, FPI, FGM, Inert Mixing, …
  - Chemistry manifold: detailed chemistry, skeletal, reduced, …
- Penalty term λ for cost/accuracy trade-off

PEC algorithmic components

- Model selection
- Error assessment
- Coupling between subzones and different models
- Computational considerations

PEC Modeling Framework
Model Selection and Error Assessment

- Model assignment $\mathcal{M} : \Omega \to M$

Physical domain

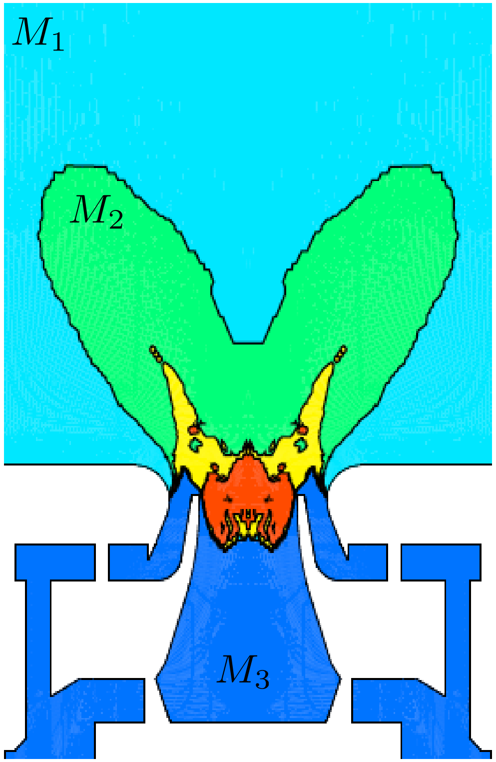
Set of candidate models {FPV, FPI, Detailed Chemistry, …}

- Solve optimization problem

$$\min_{\mathcal{M}:\Omega\to M} \mathcal{E}(\mathcal{M}) + \lambda \mathcal{C}(\mathcal{M}) \,,$$

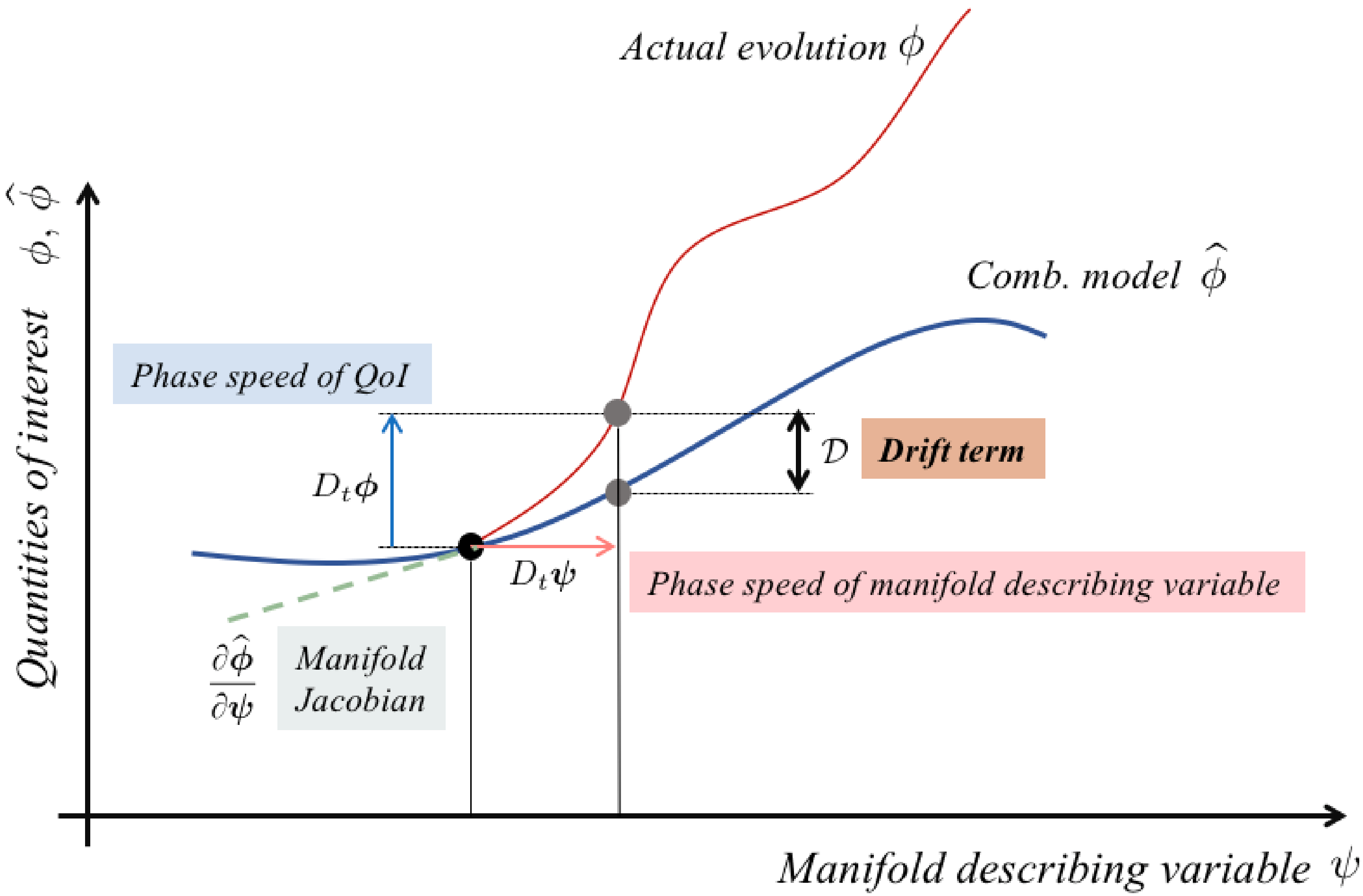
with

- Model error: $\mathcal{E}(\mathcal{M}) = \int_\Omega \left| e^{\mathcal{M}}(\mathbf{x}) \right| d\mathbf{x} \,,$
- Cost: $\mathcal{C}(\mathcal{M}) = \int_\Omega \left| c^{\mathcal{M}}(\mathbf{x}) \right| d\mathbf{x} \,.$



PEC Modeling Framework
Error Assessment – Key idea

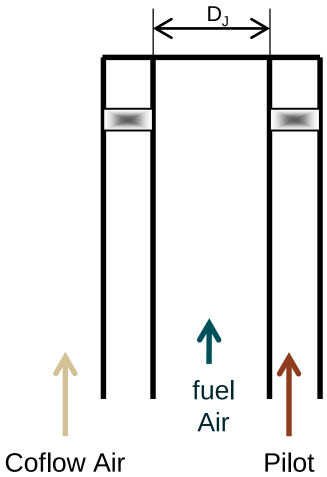
Drift term: initial growth rate of error

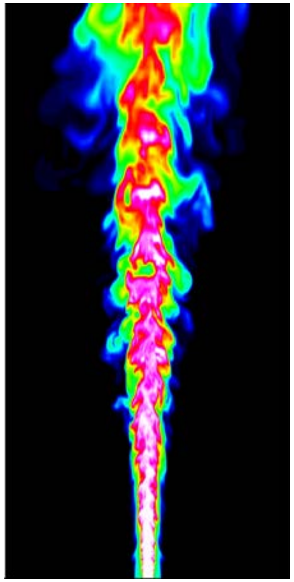


Piloted turbulent partially-premixed jet flame

DME Flame-D

- Experimental Configuration
  - Piloted partially-premixed jet flame
- Numerical Configuration
  - 10 million control volumes
  - Finite-rate chemistry: 18/44 species
  - Combustion models
    - Flamelet/progress-variable (FPV)
    - Finite-rate chemistry (FRC)
    - Adaptive model (PEC)
  - Dynamic thickened flame model

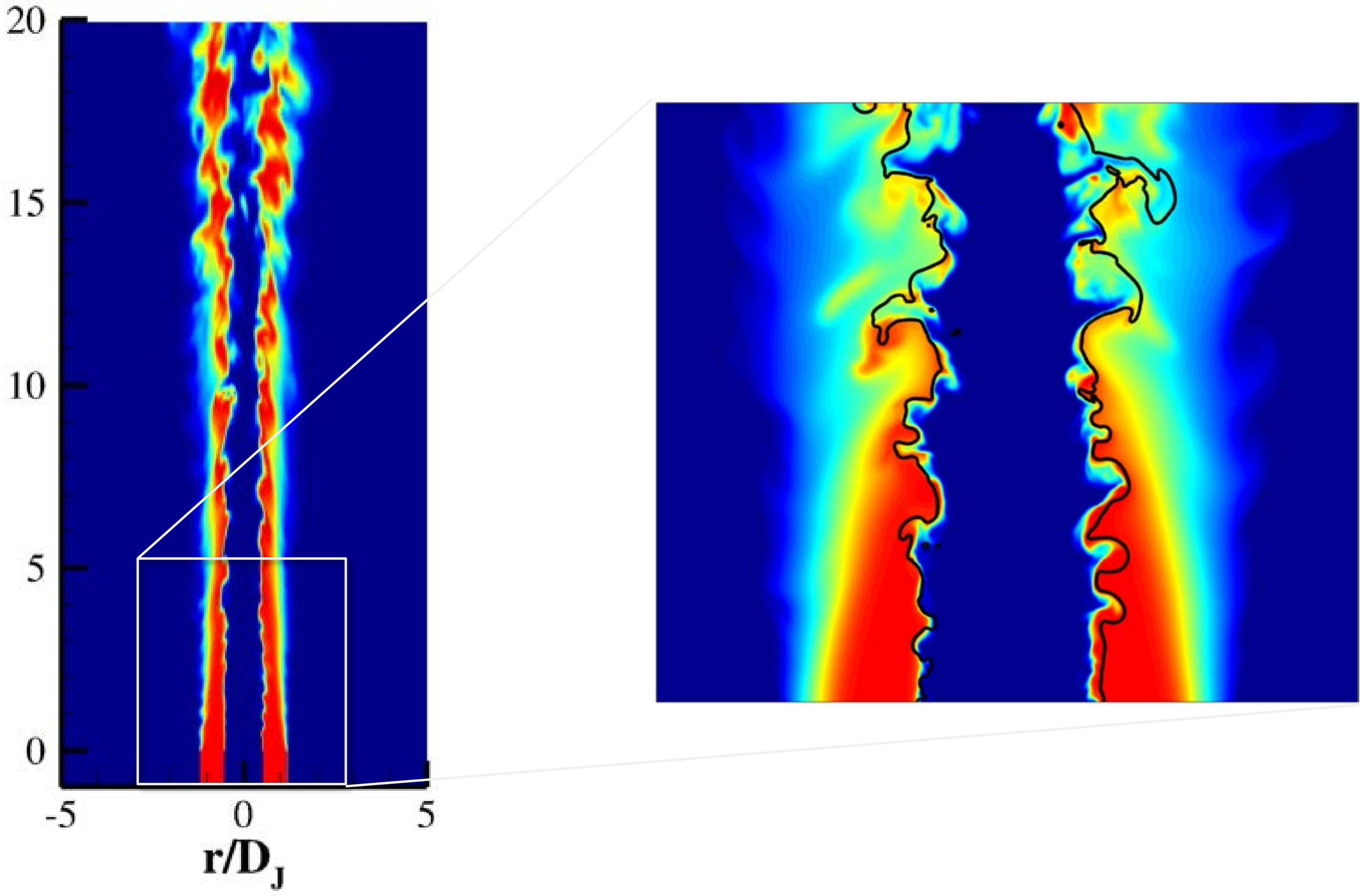




Fuest, F., Magnotti, G., Barlow, R. S., & Sutton, J. A. (2015). Scalar structure of turbulent partially-premixed dimethyl ether/air jet flames. *Proceedings of the Combustion Institute*, *35*(2), 1235-1242.

Piloted turbulent partially-premixed DME jet flame

Application of drift term to LES of Sydney flame (Lr75)



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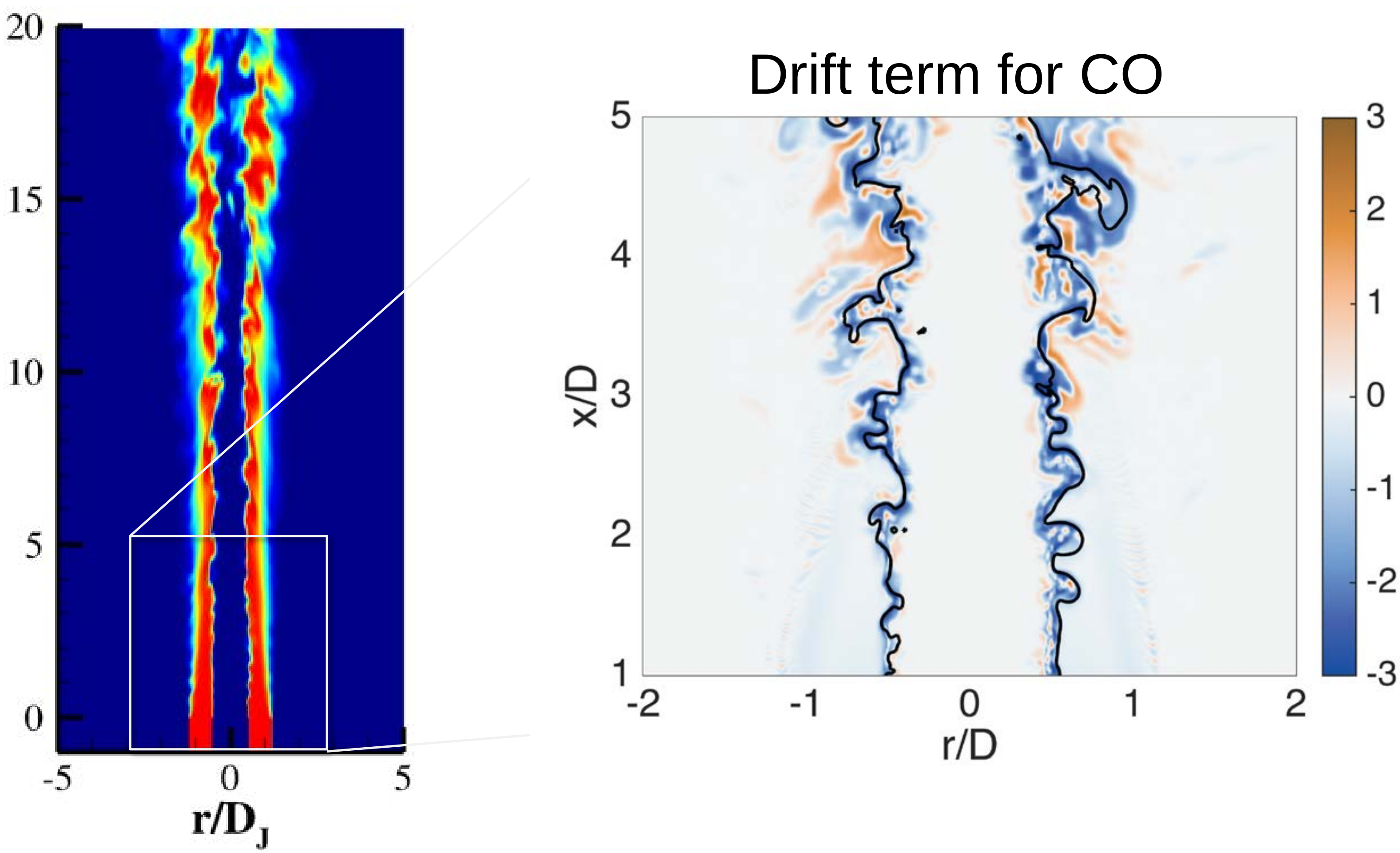

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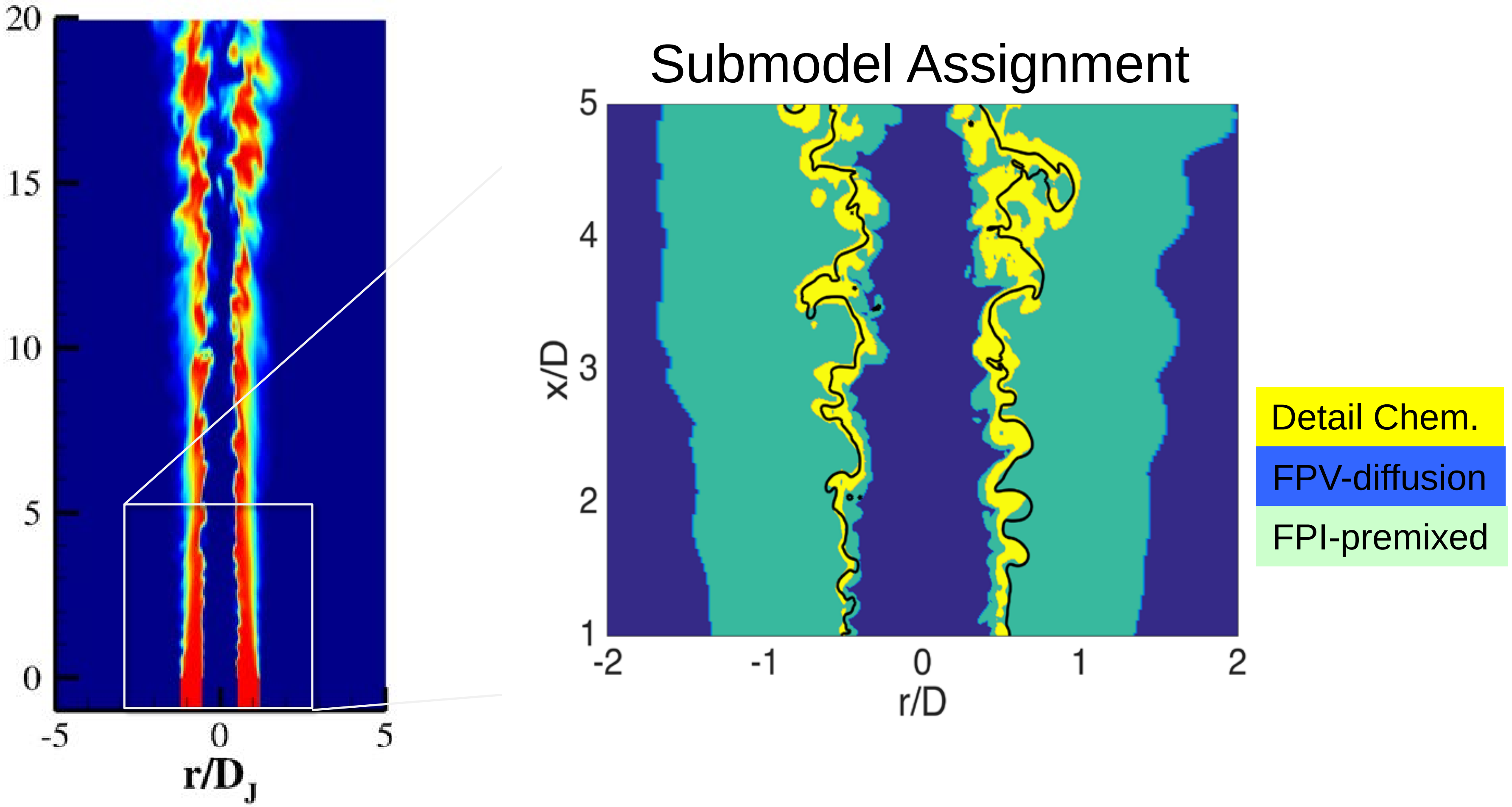
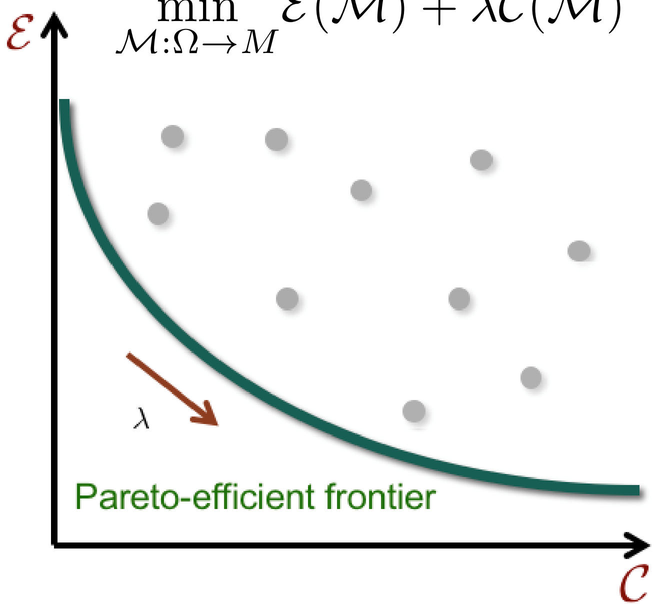


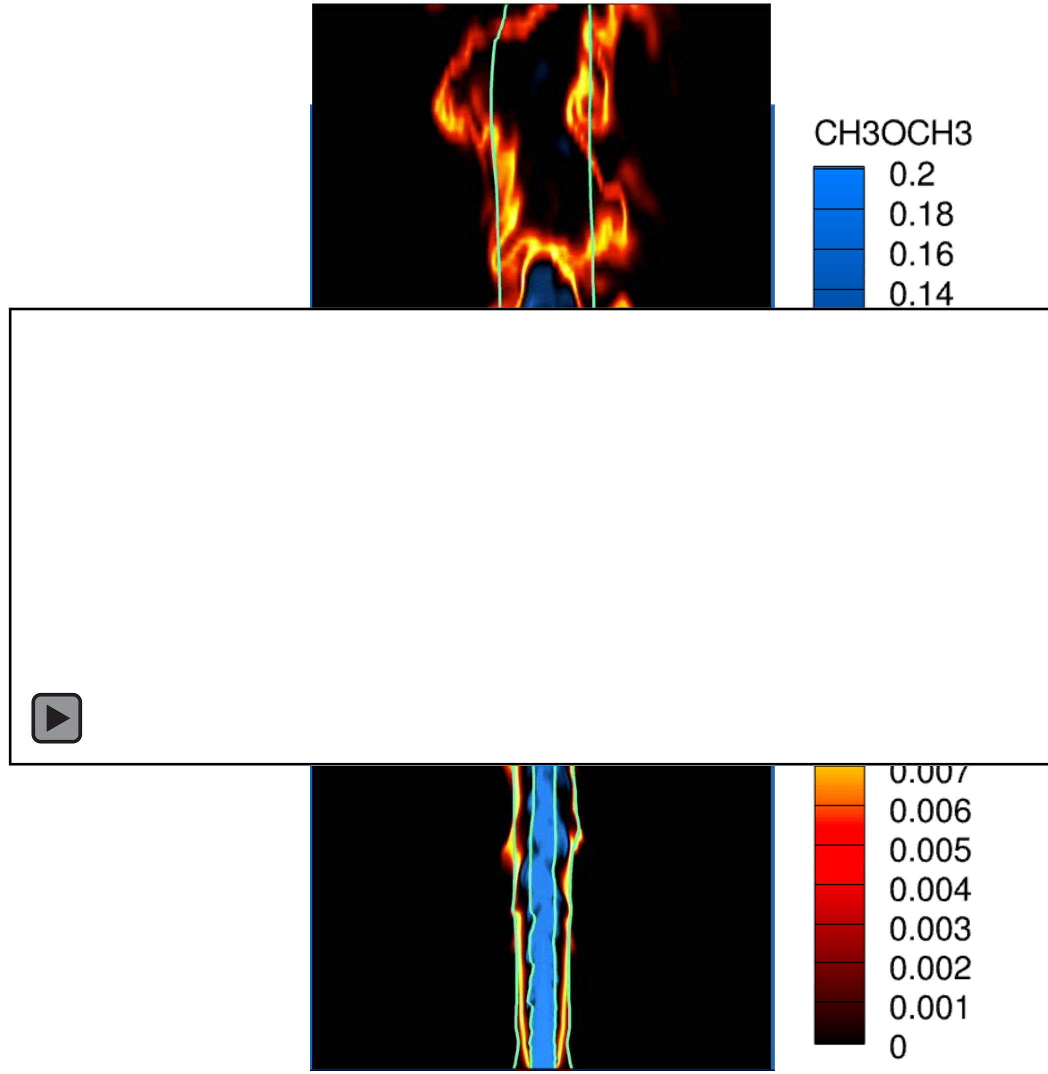
Piloted turbulent partially-premixed DME jet flame

Cases

- PEC-64 (λ = 0.64, FPV)
- PEC-8 (λ = 0.08, FPV / FRC)
- PEC-0 (λ = 0.00, FRC)

$$\min_{\mathcal{M}:\Omega\to M} \mathcal{E}(\mathcal{M}) + \lambda \mathcal{C}(\mathcal{M})$$





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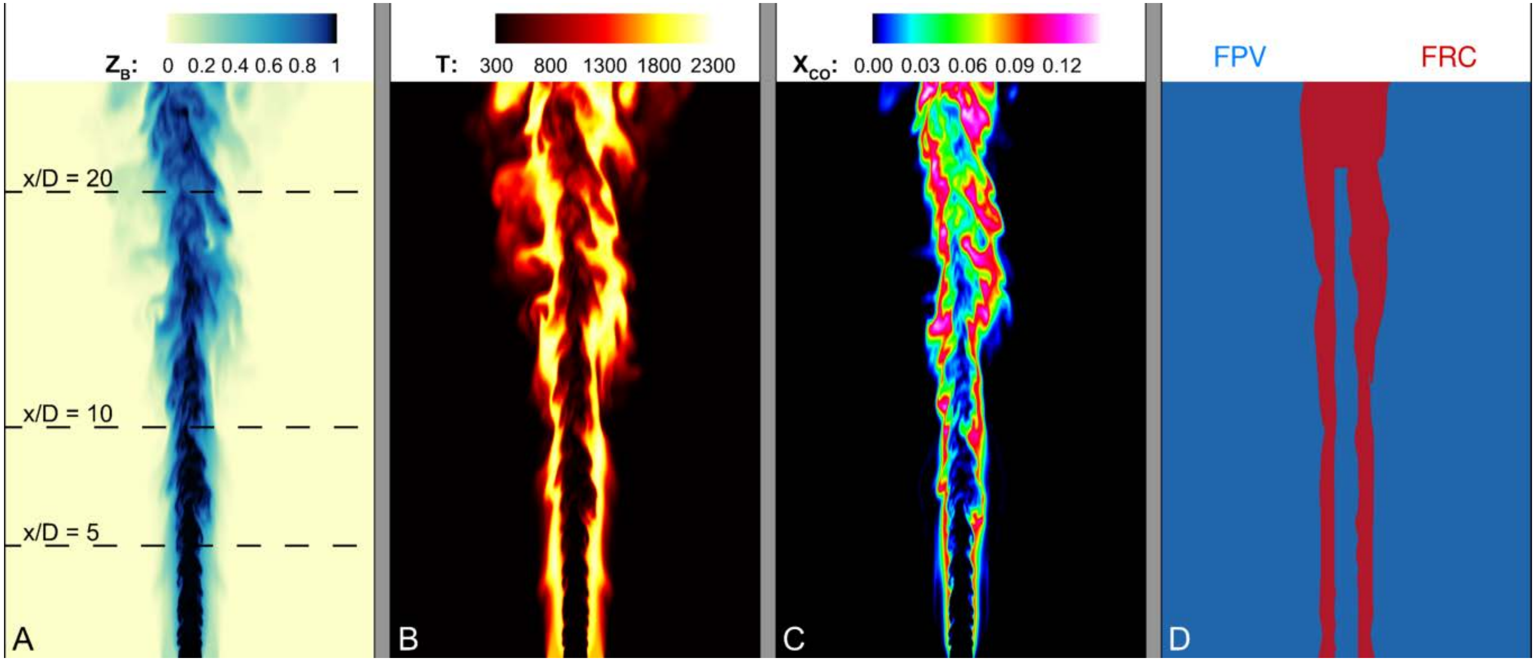
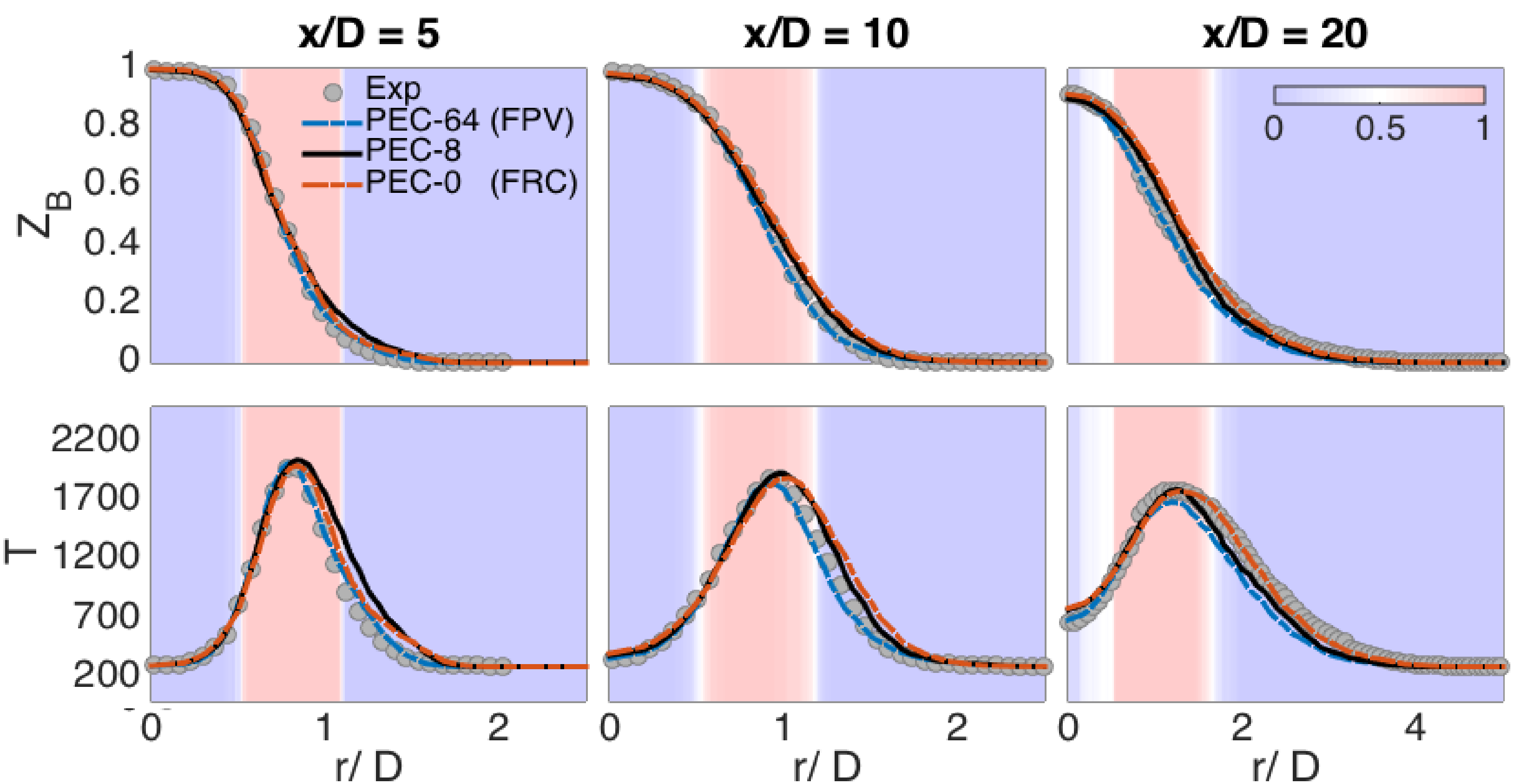


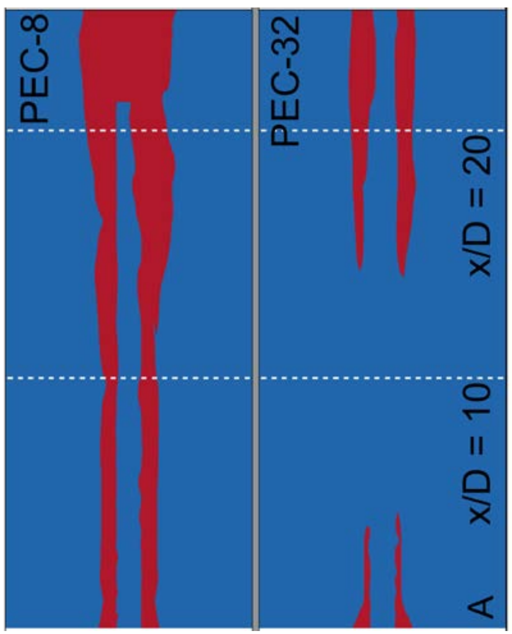
Piloted turbulent partially-premixed DME jet flame

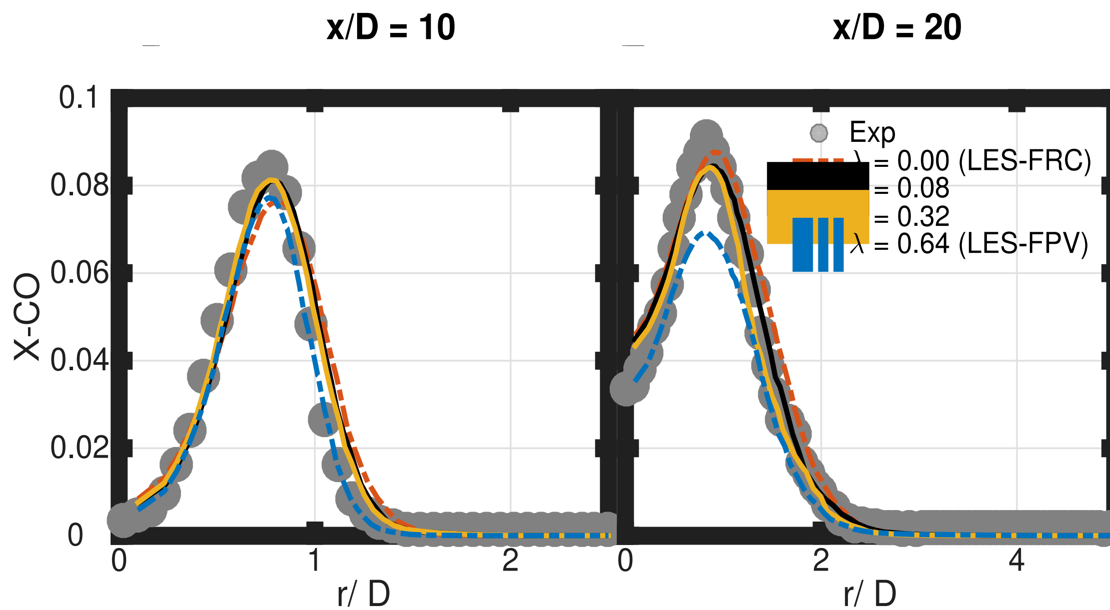
Radial profiles



Piloted turbulent partially-premixed DME jet flame

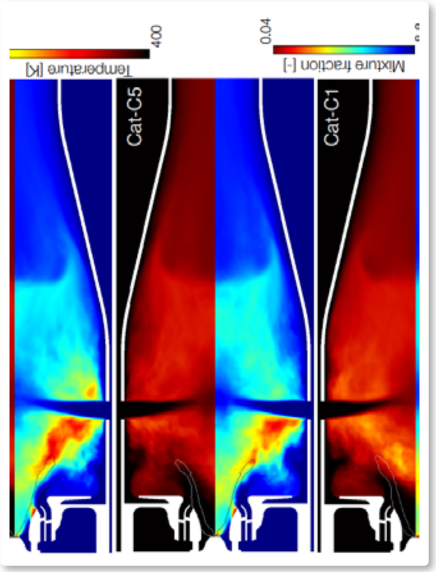
Comparison of PEC-8 and and PEC-32





Application to Complex Combustor

EVALUATION OF MODEL COMPLIANCE

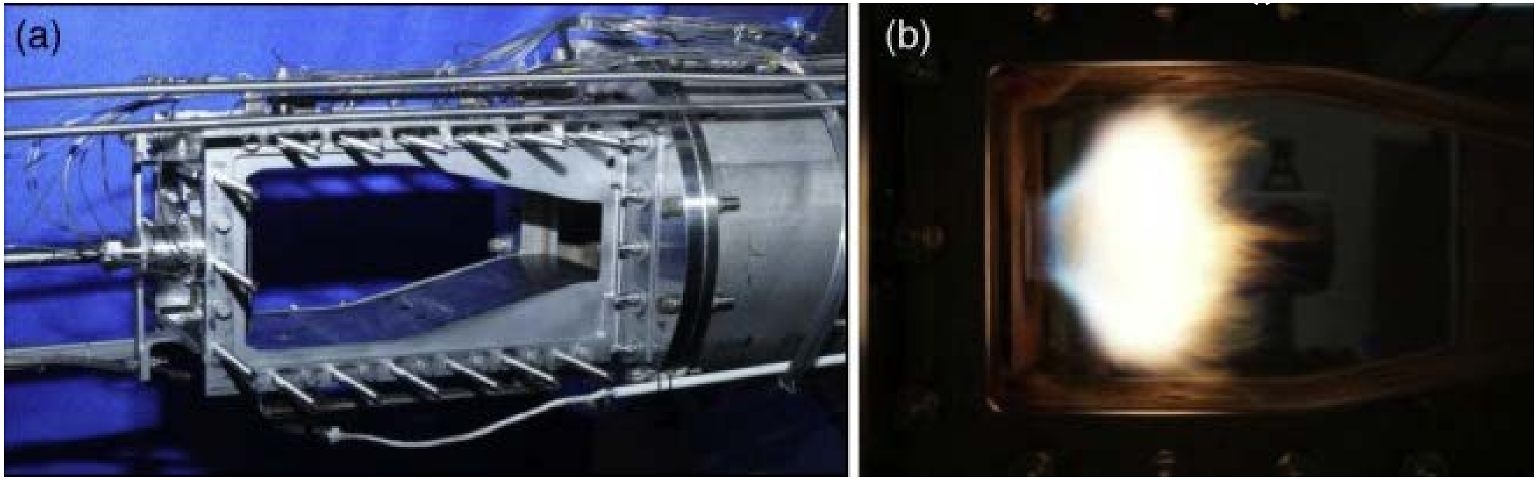


Referee gas turbine combustor

Case setup

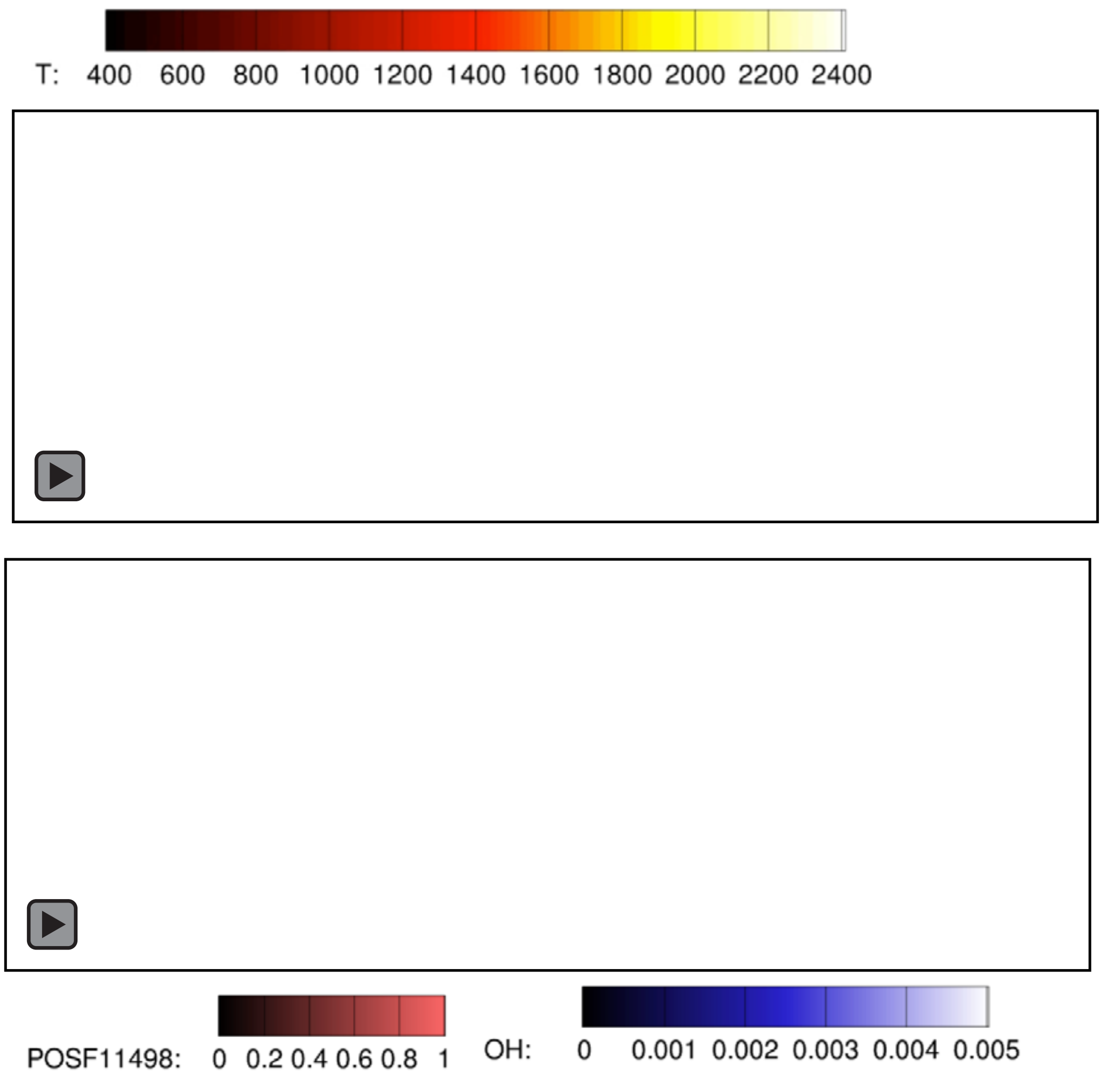
- NJFCP referee combustor
- Pressure: 2.07 bar
- Injection system with swirlers
- Fuel: Cat-C1, POSF11498 ($C_{13}H_{28}$)
- Equivalence ratio: $\phi = 0.096$

- Mesh: 26 million elements
- Chemistry: 26-species reduced mechanism**
- Candidate models:
  - › Flamelet/progress-variable (FPV)
  - › Finite-rate chemistry (FRC)
- QoI = {CO, CO_2, H_2, H_2O, CH_2O}



* Esclapez, L. et al.. (2017). *Combust Flame*, *181*.
** Gao, Y., & Lu, T. (2017). 10th U.S. National Combust. Meeting.

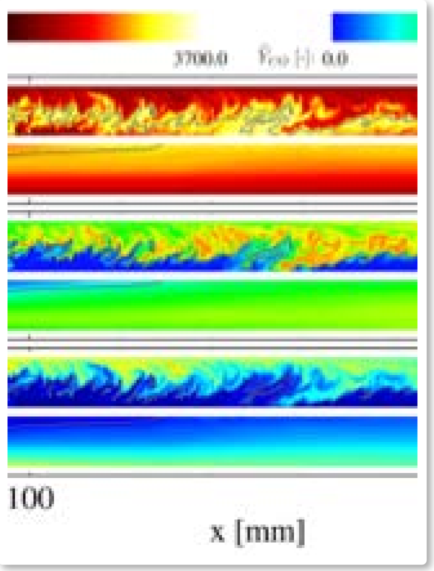
Referee gas turbine combustor



- 30% FRC ($\lambda = 2$)
- 40% reduction in cost

Limitations and Data-assisted modeling

EVALUATION OF MODEL COMPLIANCE



Motivation

- High-fidelity simulations of turbulent reacting flows can incur high computational costs
- Use Pareto-efficient Combustion (PEC) framework for submodel assignment

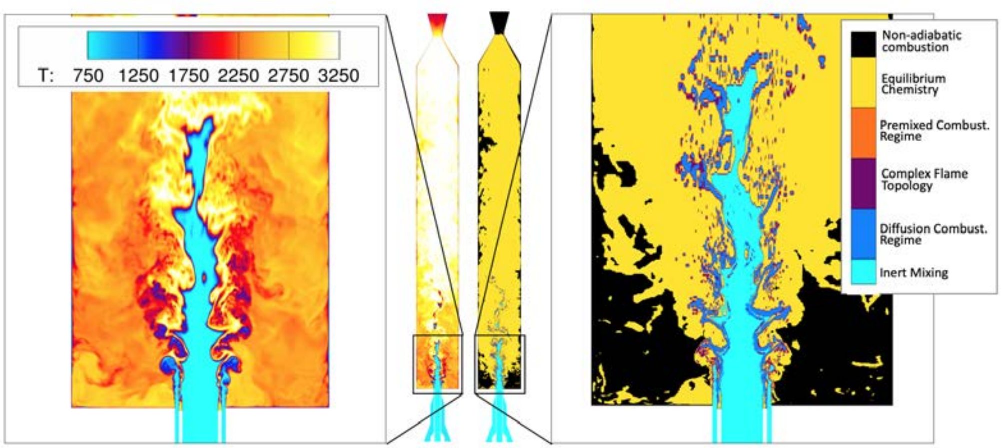


Figure 3: Combustion-mode analysis in a rocket injector.

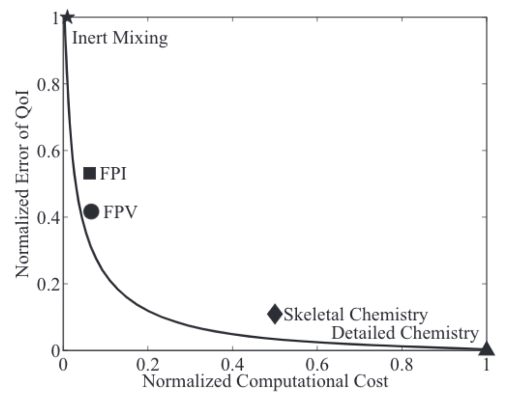
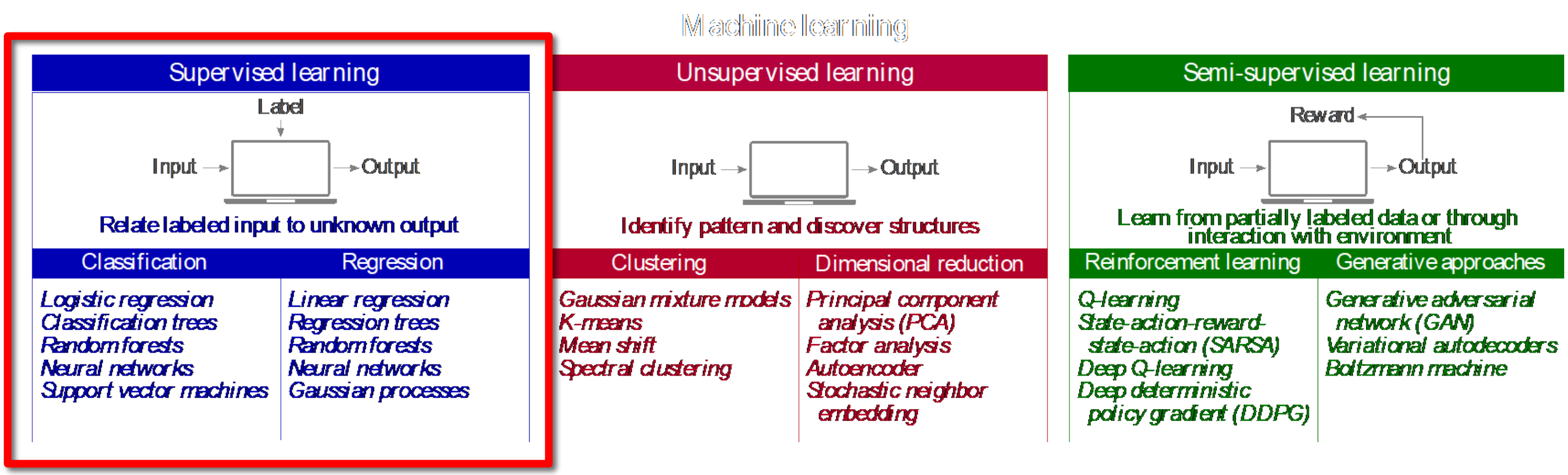


Fig. 1. Schematic illustration of the Pareto front, representing the computational cost and model error in predicting a certain quantity of interest.

Machine Learning Techniques

- PEC is mathematically rigorous but limited by reliance on local information regarding the chemical composition
- Data-driven techniques such as ML offer a generalized approach



Brunton et. al., Ann. Rev. Fluid Mech. (2020)

Problem with ML-based regression

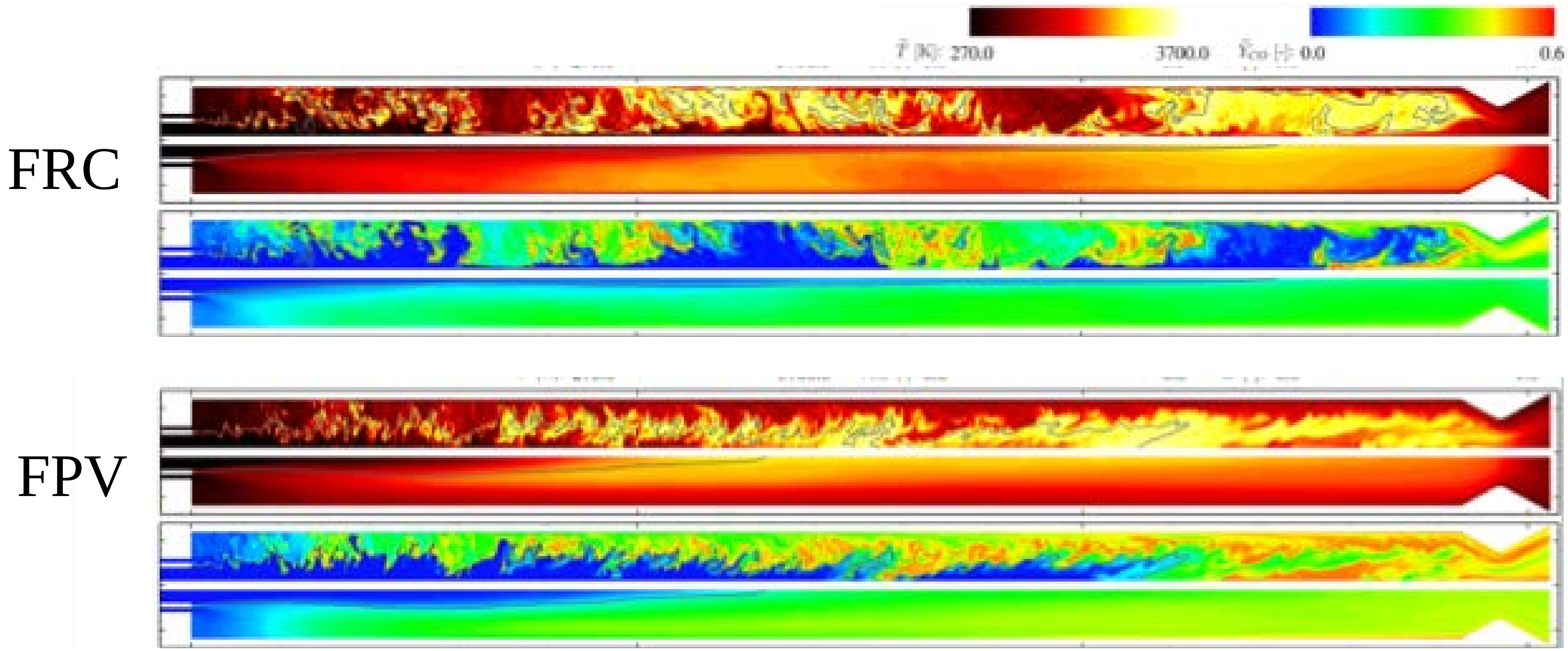
- Physical models versus data-driven models: conservation laws versus complex cross-correlations.
- Data-driven models may violate physics, especially when extrapolation occurs.
- Data driven models are prone to numerical instability.

Solution?

- Use data-driven method to **assist** the selection of low-fidelity physics-based model through classification

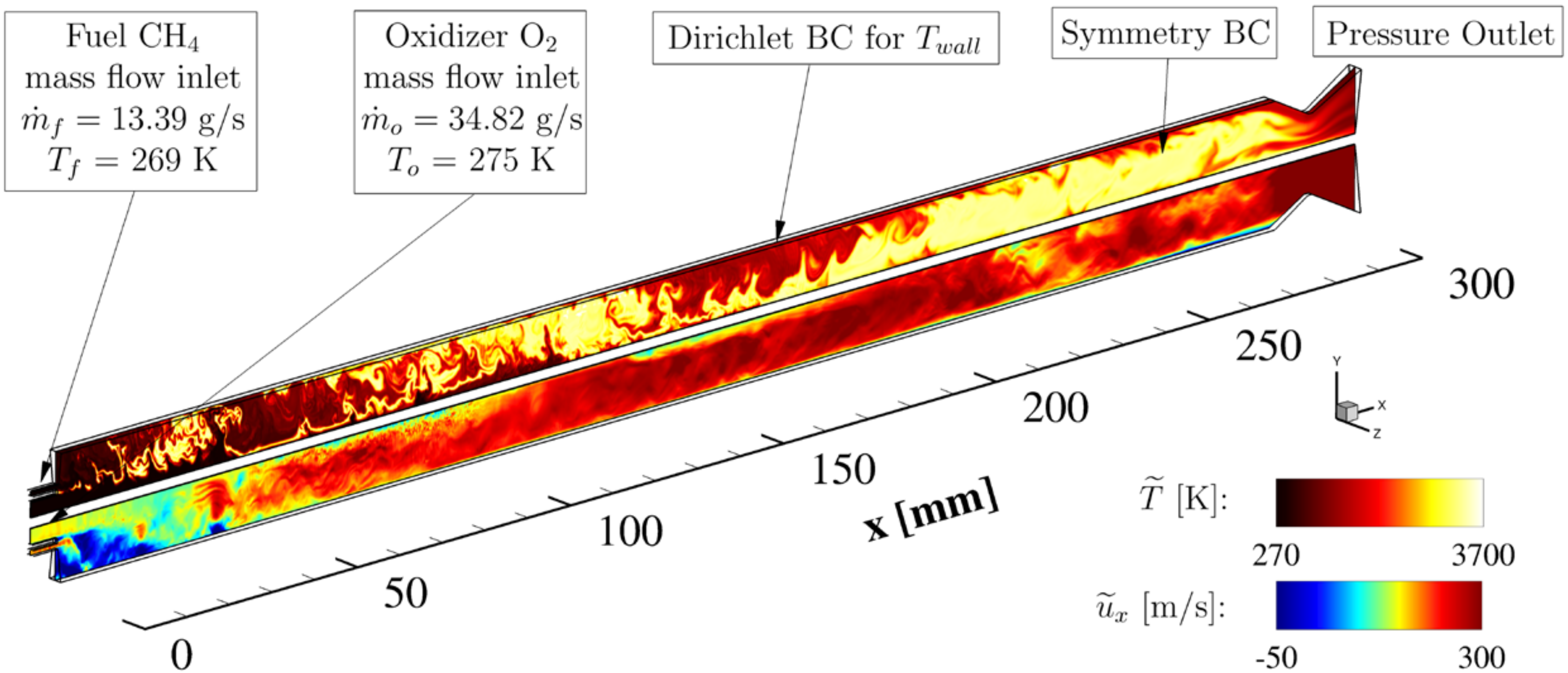
Objective

- Flamelet Progress Variable (FPV) model cannot capture thermal boundary layers
- Use ML (Random Forest) to improve on FPV simulations at a lower cost than Finite-Rate Chemistry (FRC)



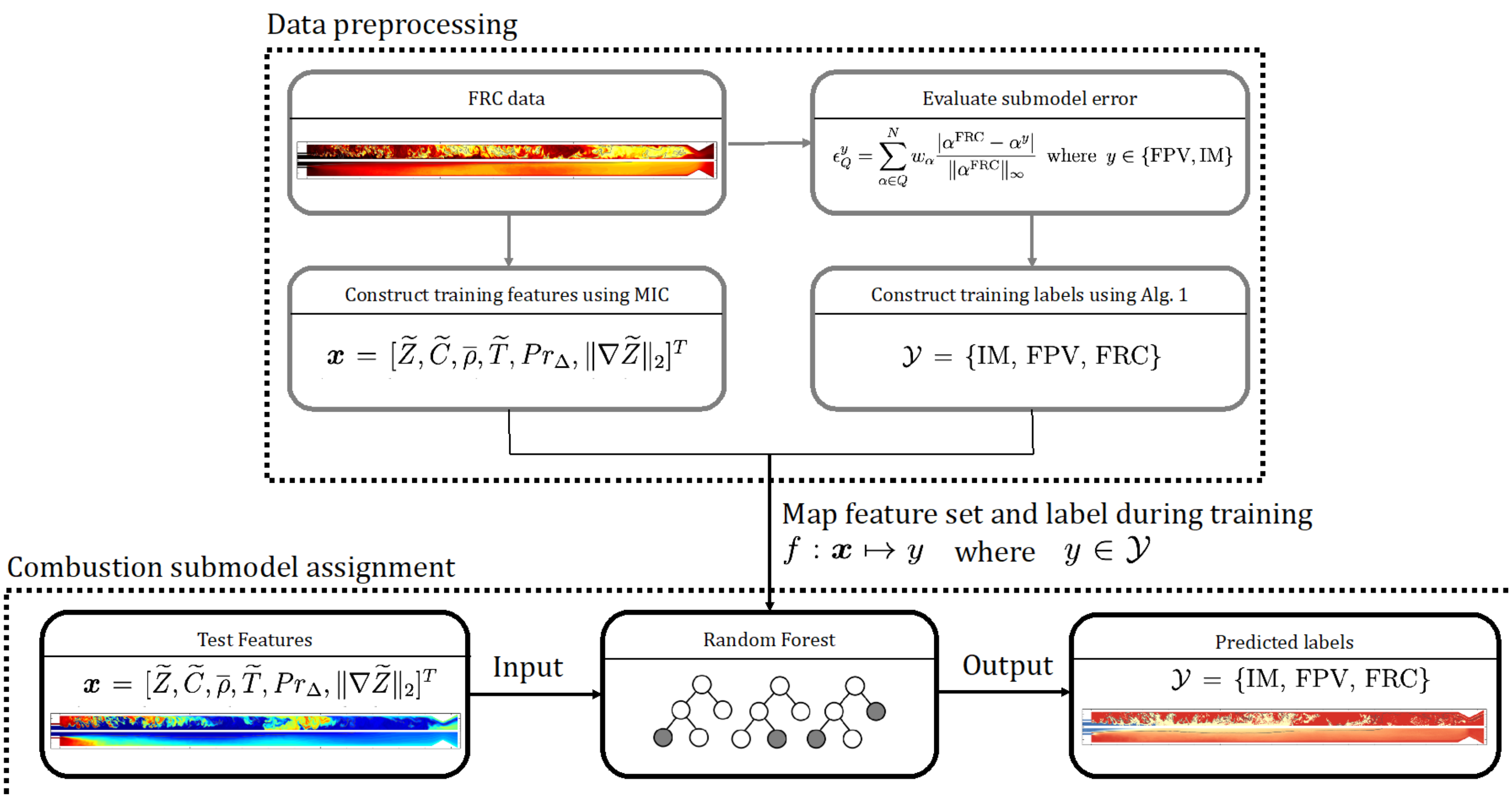
Setup

- Based on GOX/GCH4 single element rocket combustor from Silvestri et. al.
- 2×10^5 cells, axisymmetric domain, with minimum cell size of 30 µm.
- Turbulent closure with with Thickened Flame and Smagorinsky models.

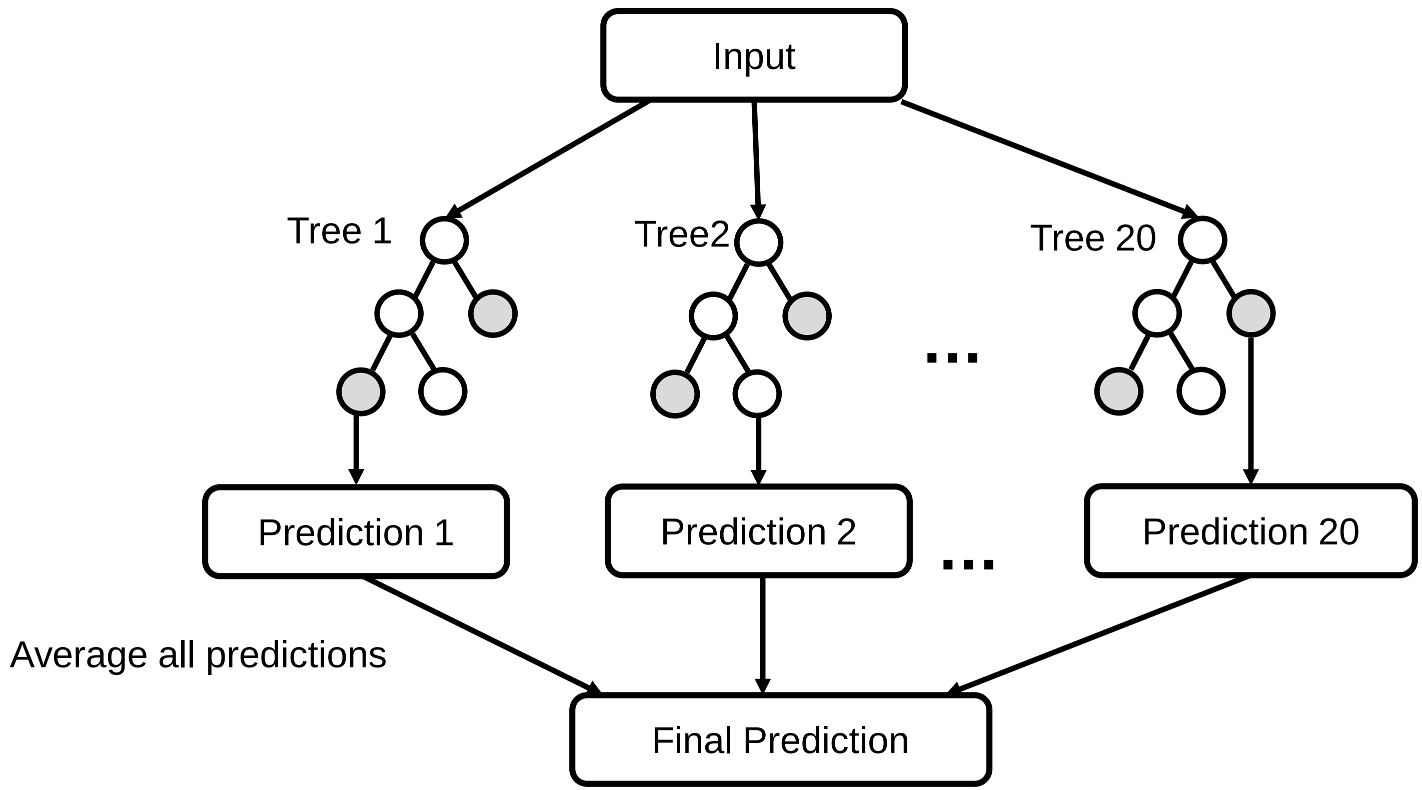


S. Silvestri, M. P. Celano, O. J. Haidn, and O. Knab, *EUCASS* (2015)

Data-assisted LES



Random forests



Constructing training labels/output

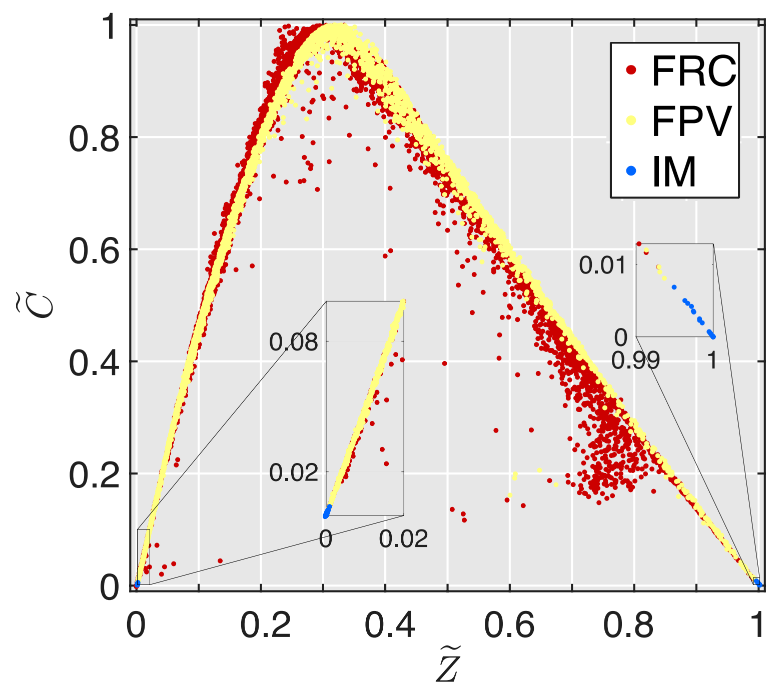
Error between different submodels for $\alpha = \{\tilde{T}, \widetilde{Y_{CO}}\}$

$$\epsilon_Q^y = \sum_{\alpha \in Q} w_\alpha \frac{|\alpha^{\mathrm{FRC}} - \alpha^y|}{\|\alpha^{\mathrm{FRC}}\|_\infty} \quad \text{with} \quad y \in \{\mathrm{FPV}, \mathrm{IM}\}$$

User defined threshold

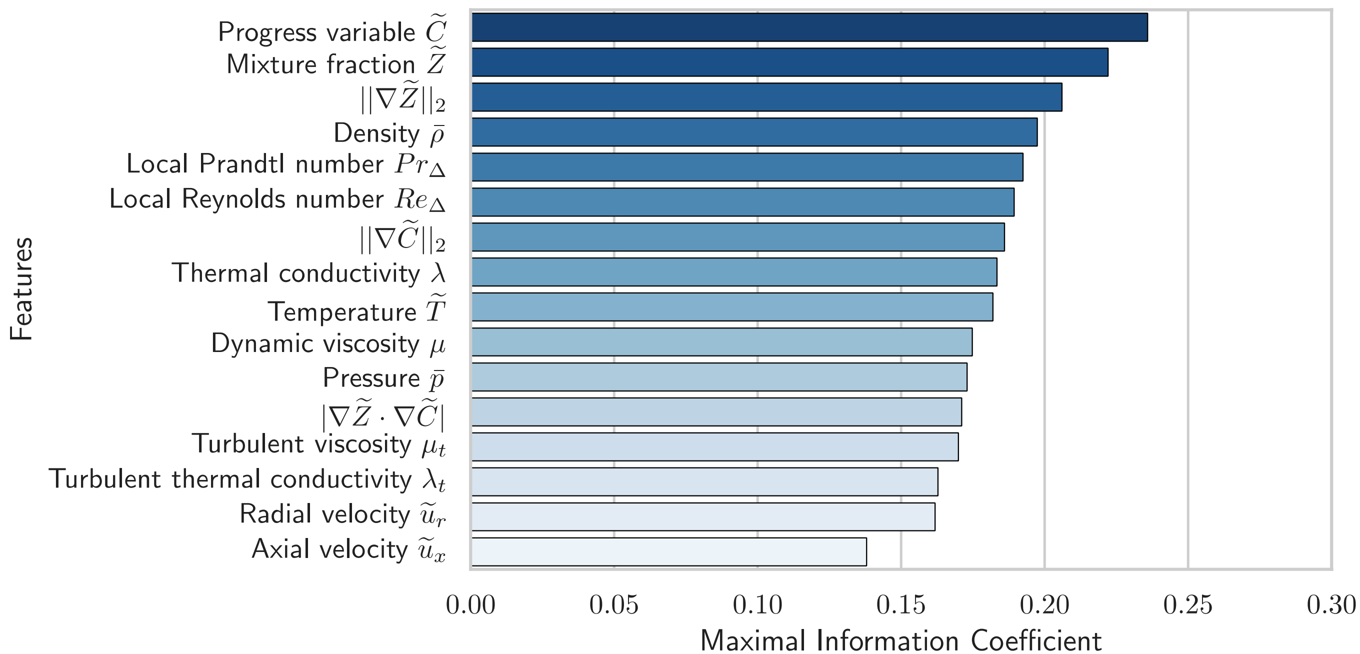
if $\epsilon_Q^{IM} < \theta_Q^{IM}$ **then**
| use inert mixing (IM)
else if $\epsilon_Q^{FPV} < \theta_Q^{FPV}$ **then**
| use tabulated chemistry (FPV)
else
| use finite-rate chemistry (FRC)
end

Training data for $\theta_{\{T,\mathrm{CO}\}} = 0.02$



Feature/input selection

- Use Maximal Information Coefficient (MIC) to select most relevant input.
- MIC is a correlation measure for nonlinear data, similar to R2 measure
- MIC relating features with $\epsilon_{\{T,CO\}}^{FPV}$

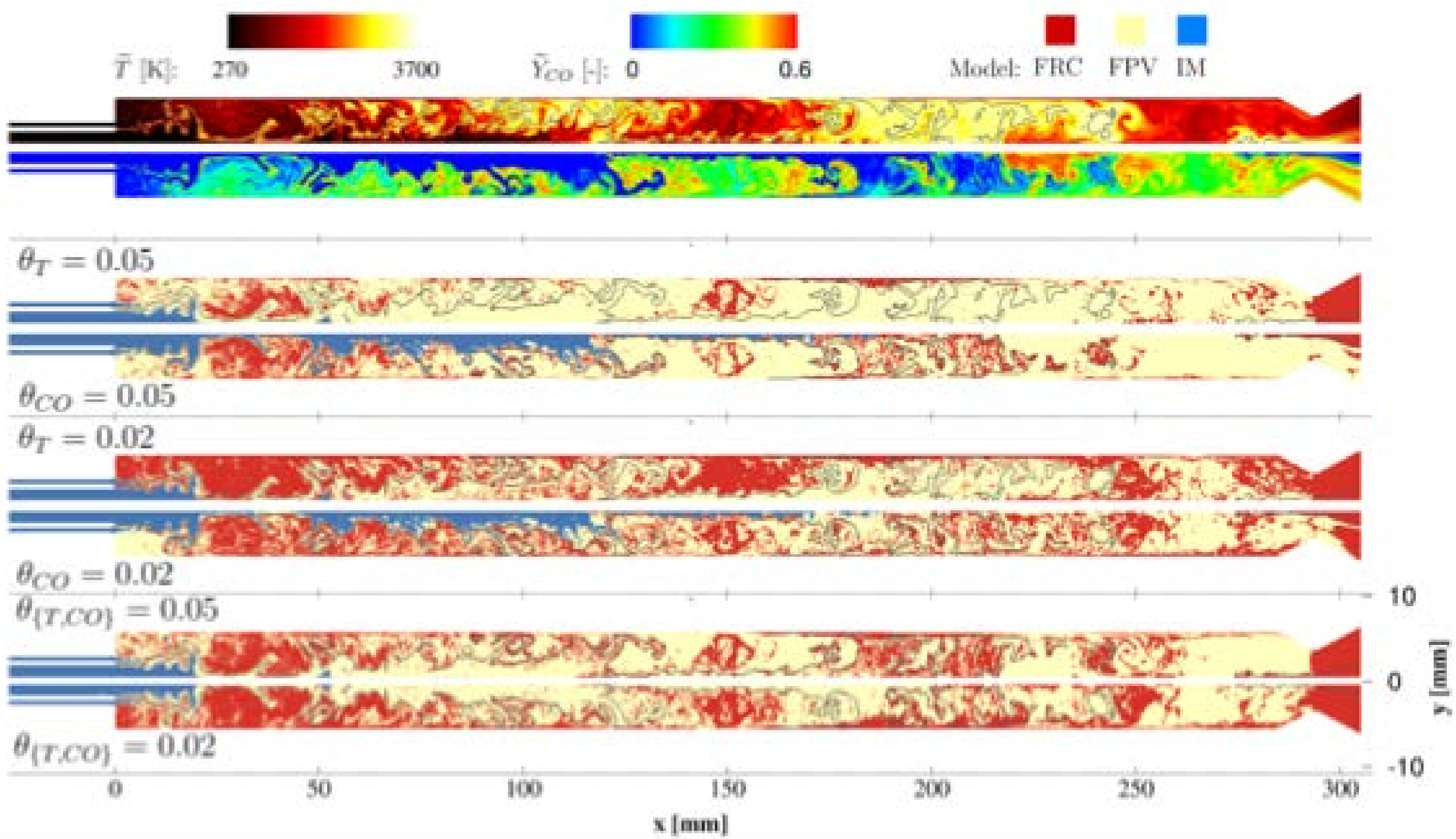


Choose top 5 features from both $\boldsymbol{x} = [\widetilde{Z}, \widetilde{C}, \bar{\rho}, \widetilde{T}, Pr_\Delta, ||\nabla\widetilde{Z}||_2]^T$

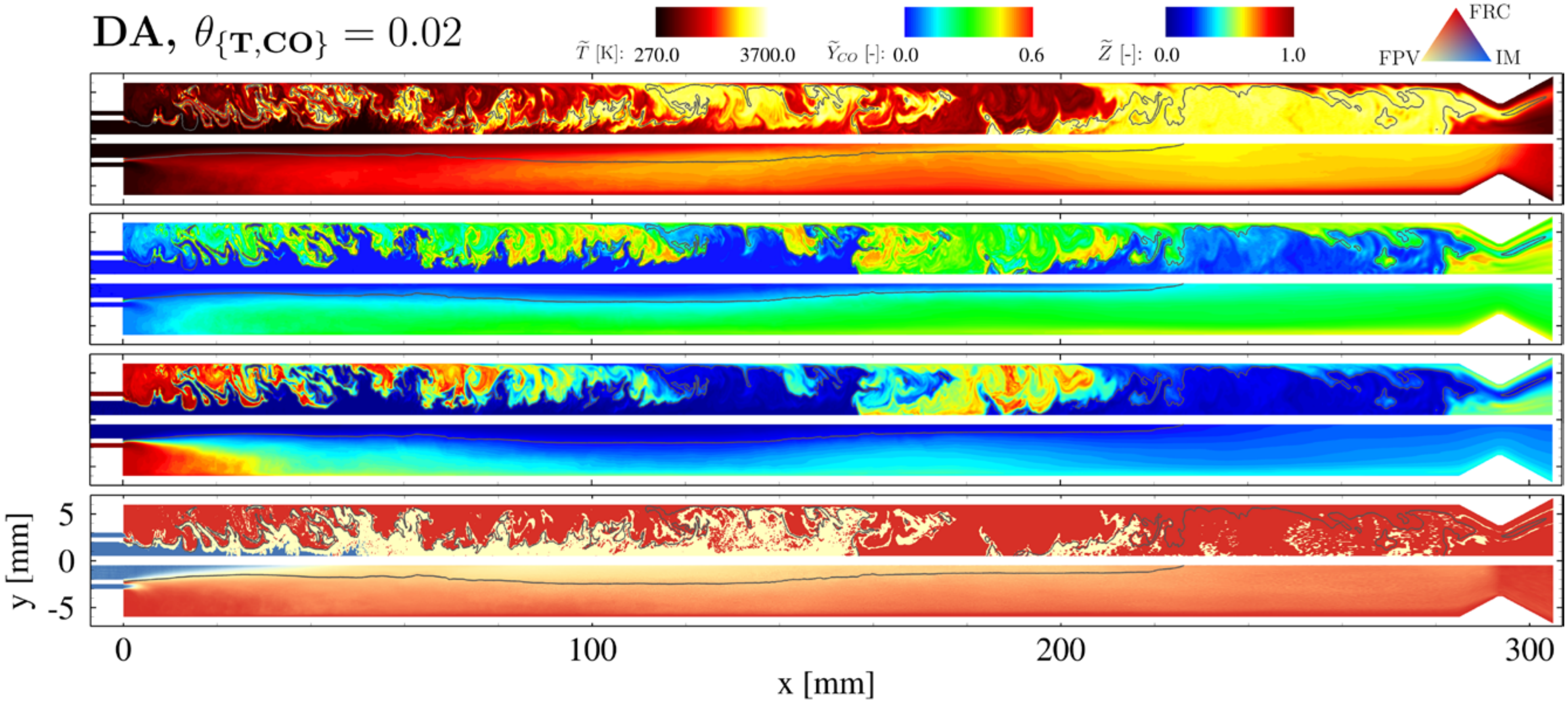
A priori results

Apply trained RF on existing FRC LES data for submodel assignment

Case	θ_T=0.05	θ_{CO}=0.05	θ_T=0.02	θ_{CO}=0.02	$\theta_{\{T,CO\}}$=0.05	$\theta_{\{T,CO\}}$=0.02
Model assignment (IM:FPV:FRC)	5:67:28	5:33:62	18:48:34	18:35:47	6:63:31	6:42:52
True Classification	0.774	0.725	0.756	0.715	0.753	0.734

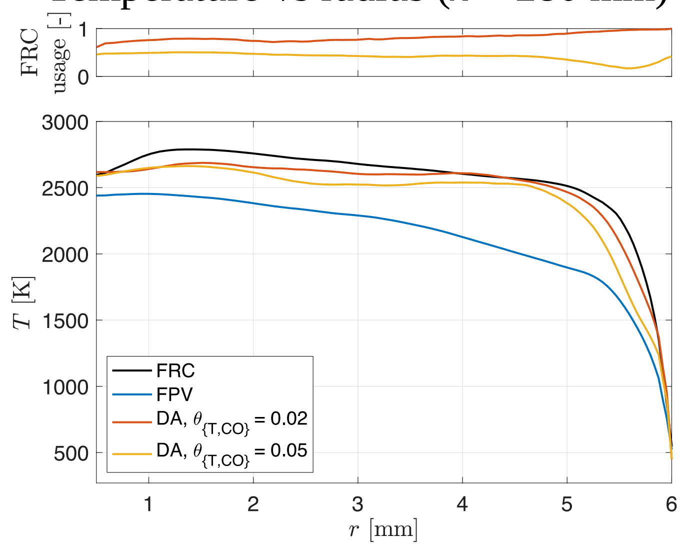


A posteriori results

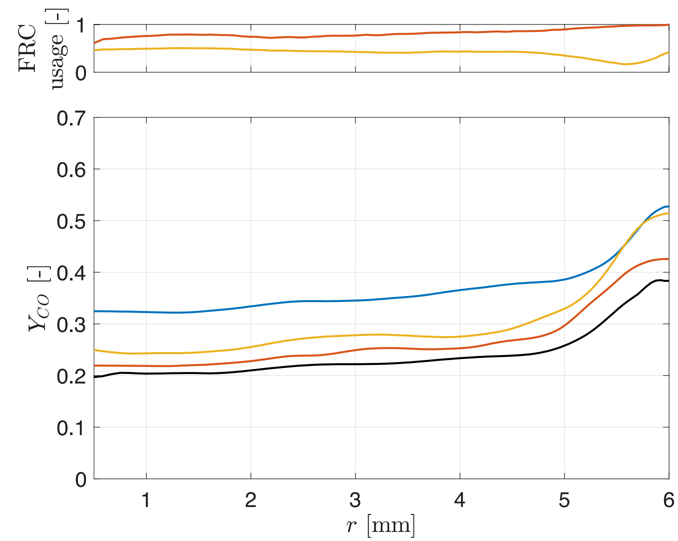


A posteriori results

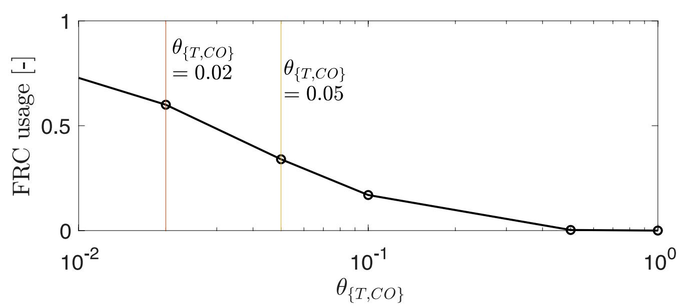
Temperature vs radius (x = 280 mm)



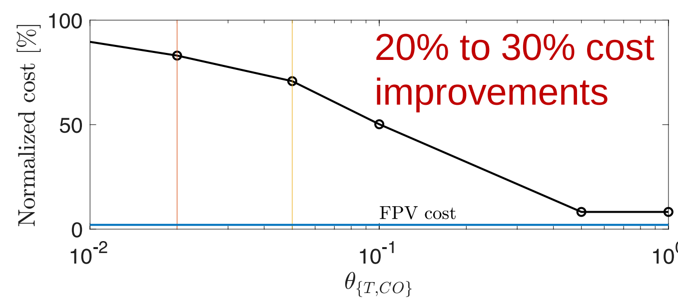
CO mass fraction vs radius (x = 280 mm)



FRC usage vs user-defined threshold

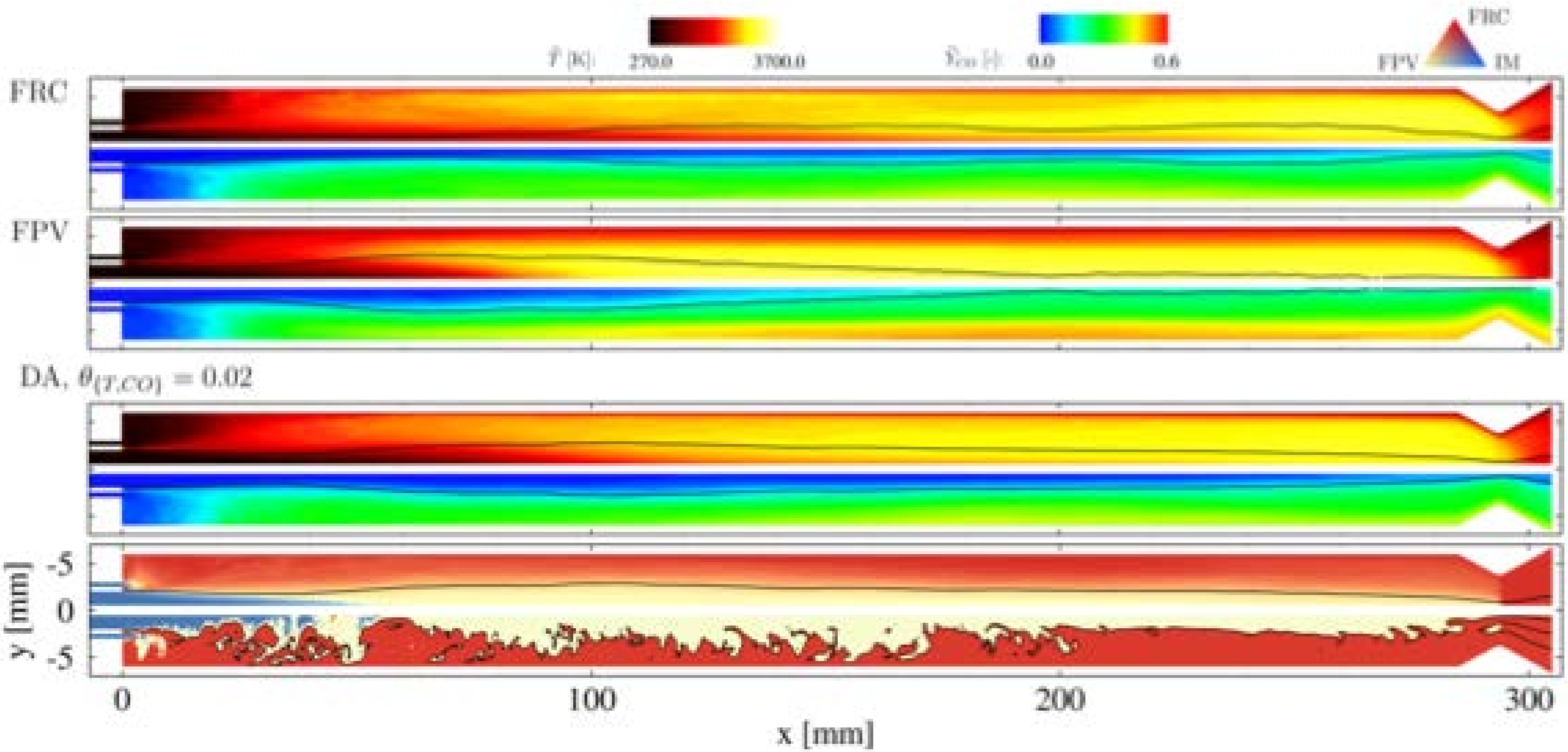


Cost vs user-defined threshold



A posteriori results (modified configuration)

- For a modified configuration with 3x inlet mass flow rate
- Method demonstrates ability to generalize for different configurations



Conclusions

- Developed a Pareto-Efficient combustion (PEC) framework for the general description of complex flame configurations
- PEC-input parameters
  - Set of quantities of interest
  - Set of candidate combustion models
  - Penalty term balancing cost and accuracy

- PEC-model components
  - Model selection
  - Error assessment → manifold drift
  - Coupling between subzones and different models

- Generalization using ML-techniques
  - Classification can be used to assign well-tested combustion models.
  - Overall desired fidelity can be controlled during labelling.
  - Data-assisted simulations outperform monolithic FPV and monolithic FRC. simulations in accuracy and cost respectively.
  - Classification ensures stability and robustness. Conservation of properties is consistent.