Random Forests for Accelerating Turbulent Combustion Simulations

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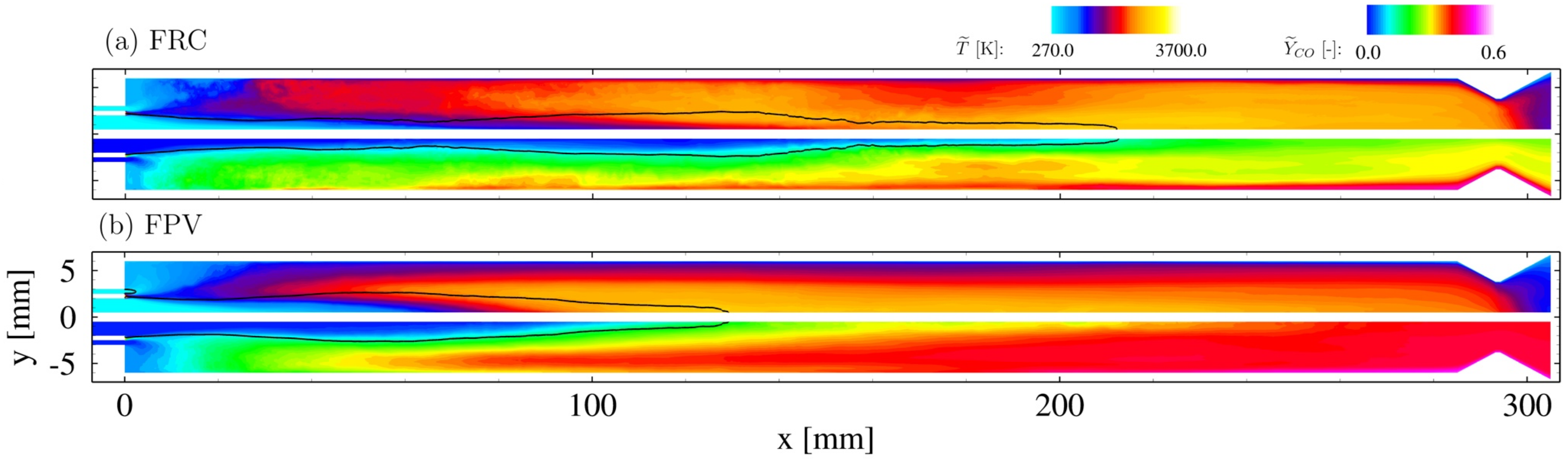
Introduction

- **Problem Statement**
  - Combustion chemistry is a computational bottleneck in high-fidelity simulations of turbulent reacting flows.
  - Low-cost models such as flamelet/progress variable (FPV) model **[1]** cannot capture thermal boundary layers and CO production, unlike costly models such as finite-rate chemistry (FRC).



- **Solution**
  - Employ classification algorithm for optimal assignment **[2]** of combustion submodels (of varying cost and fidelity) in the simulation domain.

Configuration and Simulation Method

- Gaseous oxygen-gaseous methane rocket combustor based on experiment [3].
- Employed a 4th order finite volume for solving Favre-filtered mass, momentum, species, and energy conservation equations:

$$\partial_t \bar{\rho} + \nabla \cdot (\bar{\rho}\widetilde{\boldsymbol{u}}) = 0 \tag{1a}$$

$$\partial_t (\bar{\rho}\widetilde{\boldsymbol{u}}) + \nabla \cdot (\bar{\rho}\widetilde{\boldsymbol{u}}\widetilde{\boldsymbol{u}}) = -\nabla \cdot (\bar{p}\boldsymbol{I}) + \nabla \cdot (\overline{\boldsymbol{\tau}}_v + \overline{\boldsymbol{\tau}}_t) \tag{1b}$$

$$\partial_t (\bar{\rho}\widetilde{e}) + \nabla \cdot [\widetilde{\boldsymbol{u}}(\bar{\rho}\widetilde{e} + \bar{p})] = -\nabla \cdot (\overline{\boldsymbol{q}}_v + \overline{\boldsymbol{q}}_t) + \nabla \cdot [(\overline{\boldsymbol{\tau}}_v + \overline{\boldsymbol{\tau}}_t) \cdot \widetilde{\boldsymbol{u}}] \tag{1c}$$

$$\partial_t (\bar{\rho}\widetilde{\boldsymbol{\phi}}) + \nabla \cdot (\bar{\rho}\widetilde{\boldsymbol{u}}\widetilde{\boldsymbol{\phi}}) = -\nabla \cdot (\overline{\boldsymbol{J}}_v + \overline{\boldsymbol{J}}_t) + \overline{\boldsymbol{S}} \tag{1d}$$

References

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Data-assisted Large-eddy Simulation

1. Generate labels using weighted normalized quantity-of-interest submodel error:

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

$$\epsilon_Q^y = \frac{1}{N}\sum_{\alpha \in Q} \frac{|\alpha^{\mathrm{FRC}} - \alpha^y|}{\|\alpha^{\mathrm{FRC}}\|_\infty} \quad \text{with } y \in \{\mathrm{FPV}, \mathrm{IM}\}, \quad Q = \{\widetilde{T}, \widetilde{Y}_{\mathrm{CO}}\}$$

θ_Q^y is a user defined threshold.

2. Select features (mixture fraction, progress variable, density, local Prandtl number, and Euclidean norm of the mixture fraction gradient) using Maximal Information Coefficient **[4]**: $\boldsymbol{x} = [\widetilde{Z}, \widetilde{C}, \bar{\rho}, \widetilde{T}, Pr_\Delta, \|\nabla \widetilde{Z}\|_2]$
3. Train, validate, and test random forests. Integrate random forest with simulation solver.

Results

- High classification accuracy when testing random forest on an unseen snapshot.

Table 1: Classification accuracy and submodel assignment of cases investigated.

Case,	θ_T=0.05	θ_{CO}=0.05	θ_T=0.02	θ_{CO}=0.02	$\theta_{\{T,\mathrm{CO}\}}$=0.05	$\theta_{\{T,\mathrm{CO}\}}$=0.02
Quantity-of-interest, Q	$\widetilde{T}$	$\widetilde{Y}_{\mathrm{CO}}$	$\widetilde{T}$	$\widetilde{Y}_{\mathrm{CO}}$	$\{\widetilde{T}, \widetilde{Y}_{\mathrm{CO}}\}$	$\{\widetilde{T}, \widetilde{Y}_{\mathrm{CO}}\}$
Classification accuracy	0.774	0.756	0.725	0.715	0.753	0.734
IM:FPV:FRC	5:67:28	18:48:34	5:33:62	18:35:47	6:63:31	6:42:52

- Employing random forests in-flight during simulation runtime captures all quantity-of-interests (temperature, CO) at **30% lower costs** than FRC.