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

Configuration and Simulation Method

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

\[
\begin{align*}
\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) &= 0 \\
\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla \cdot (\rho \mathbf{f}) + \nabla \cdot (\rho \mathbf{v} + \mathbf{f}) \\
\partial_t (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v} + \rho \\mathbf{u}) &= -\nabla \cdot (\rho \mathbf{v} + \rho \mathbf{f}) + \nabla \cdot (\rho \mathbf{v} + \rho \mathbf{f}) \\
\partial_t (\rho \mathbf{w}) + \nabla \cdot (\rho \mathbf{w} \mathbf{w} + \rho \\mathbf{u}) &= -\nabla \cdot (\rho \mathbf{w} + \rho \mathbf{f}) + \nabla \cdot (\rho \mathbf{w} + \rho \mathbf{f})
\end{align*}
\]

Data-assisted Large-eddy Simulation

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

\[
e_Q^p = \frac{1}{N} \sum_{n \in Q} \frac{|a^{\text{FRC}} - a^{\text{FPV}}|}{a^{\text{FRC}} + a^{\text{FPV}}} \text{ with } y \in \{\text{FPV, IM}\} , Q = \{\tilde{T}, \tilde{Y}_{CO}\}
\]

2. Select features (mixture fraction, progress variable, density, local Prandtl number, and Euclidean norm of the mixture fraction gradient) using Maximal Information Coefficient [4]:

\[
x = [\tilde{Z}, \tilde{C}, \tilde{p}, \tilde{T}, Pr_{\Delta}, \|\nabla \tilde{Z}\|_2]
\]

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>
<thead>
<tr>
<th>Case,</th>
<th>(\theta_T=0.05)</th>
<th>(\theta_{\text{CO}}=0.05)</th>
<th>(\theta_T=0.02)</th>
<th>(\theta_{\text{CO}}=0.02)</th>
<th>(\theta_T,\theta_{\text{CO}}=0.05)</th>
<th>(\theta_T,\theta_{\text{CO}}=0.02)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity-of-interest, (Q)</td>
<td>(\tilde{T})</td>
<td>(\tilde{Y}_{CO})</td>
<td>(\tilde{T})</td>
<td>(\tilde{Y}_{CO})</td>
<td>(\tilde{T}, \tilde{Y}_{CO})</td>
<td>(\tilde{T}, \tilde{Y}_{CO})</td>
</tr>
<tr>
<td>Classification accuracy</td>
<td>0.774</td>
<td>0.756</td>
<td>0.735</td>
<td>0.715</td>
<td>0.753</td>
<td>0.734</td>
</tr>
</tbody>
</table>

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

References