latentBatchSMOKE++, a latent variable transport solver for batch reactors with detailed chemistry computation

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Abstract

Combustion is a complex, multi-scale process involving intricate physical phenomena that make its simulation highly demanding in terms of computational resources. To address these challenges, reduced-order models are critical for both enhancing our understanding and accelerating simulations. This study presents a latent variable transport framework tailored for efficient simulation of 0D batch reactors. To further improve solver performance, a projected tolerance strategy is introduced, offering robustness across varying score scalings.

The approach is tested on the combustion of methane, propane, and n-heptane, using both detailed and lumped kinetic mechanisms. Results show that projected tolerances outperform fixed tolerances by preserving accuracy while significantly reducing computation time and the number of solver steps. The influence of the kinetic mechanism type is also examined: the latent solver yields greater efficiency gains with detailed mechanisms, owing to their higher species count and lower stiffness, whereas lumped mechanisms, despite being simpler, present higher stiffness that limits computational benefits.

Overall, the proposed method provides an effective balance between accuracy and efficiency, and represents a valuable strategy for reduced-order modeling in combustion research.

Introduction

Combustion is a complex, multi-scale phenomenon that makes simulations computationally intensive. Reduced-order models (ROMs) are crucial for accelerating simulations and enhancing understanding. This work focuses on linear techniques that transform the original state variables into latent variables (LVs), with Principal Component Analysis (PCA) being a widely used method due to its ability to retain maximum variance and produce orthogonal components.

Building on the PCA-based framework introduced by Sutherland and Parente [1], where transport equations are solved for principal components (PCs) instead of the original variables, a key limitation has been identified in the literature: the non-linear relationship between the state space and the source terms. This non-linearity often necessitates a large number of PCs to accurately reconstruct source terms, thereby limiting potential computational speed-ups.

In this work, we propose an optimized linear latent variable transport method with direct computation of the source terms. This approach achieves substantial computational savings while maintaining high accuracy, marking a significant advancement in linear ROMs for combustion modeling.

Materials and methods

The latentBatchSMOKE++ solver, built on OpenSMOKE++ [2], implements latent variable (LV) transport for batch reactors under non-isothermal, constant pressure conditions.

Chemical reactions are modeled in the latent space through an ODE system of the form $\frac{\partial \rho \mathbf{z}_j}{\partial t} = \mathbf{S}_{\mathbf{Z}_\mathrm{j}}$, where $\mathbf{z}_\mathrm{j}$ is the j-th latent variable and $\mathbf{S}_{\mathbf{Z}_\mathrm{j}}$ its corresponding source term. The solver allows for both positive and negative LVs without fixed bounds, using wide numerical limits ([-10^{12}, 10^{12}]) to maintain stability. Although this approach delivers accurate results, it has not been specifically optimized for LVs, which often differ significantly in magnitude from species concentrations.

The accuracy of the ODE solver depends on parameters such as tolerances, step size, and integration order. Traditionally, **fixed tolerances** are used by adapting species tolerances $\boldsymbol{\epsilon}(\boldsymbol{\Phi}) = \epsilon_a^{\Phi} + \epsilon_r^{\Phi}\boldsymbol{\Phi}$, to the latent space $\boldsymbol{\epsilon}(\mathbf{Z}) = \epsilon_a^{\Phi} + \epsilon_r^{\Phi}|\mathbf{Z}|$, ensuring positivity via the absolute value. This work introduces **projected tolerances**, which better reflect the scale of latent variables: $\boldsymbol{\epsilon}(\mathbf{Z}) = \boldsymbol{\epsilon}_{\boldsymbol{a}}^{\mathbf{Z}} + \boldsymbol{\epsilon}_{\boldsymbol{r}}^{\mathbf{Z}}|\mathbf{Z}|$, where $\boldsymbol{\epsilon}_{\boldsymbol{a}}^{\mathbf{Z}} = |(\epsilon_a^{\Phi} + \epsilon_r^{\Phi})\boldsymbol{D}^{-\mathbf{1}}\boldsymbol{A}|$ and $\boldsymbol{\epsilon}_{\boldsymbol{r}}^{\mathbf{Z}} = \boldsymbol{\epsilon}_{\boldsymbol{r}}^{\boldsymbol{\Phi}}$. These are obtained by projecting species tolerances into the latent space, yielding improved consistency between the original and reduced representations.

Results

The latent batch reactor is evaluated using three fuel/air mixtures: CH4, C3H8, and NC7H16. Modified kinetic mechanisms excluding Ar and He are employed: a 251-species mechanism for methane and propane [3], and LLNL mechanism 3.1 for n-heptane, which includes 654 species [4]. The training data comprises 99 unique reactor configurations with initial temperatures ranging from 1400 and 1500K, and equivalence ratios between 0.7 and 1.1. The base is calculated via PCA and the simulations are performed on 56 test points, 45% of which were not included in the training set.

Figure 1 compares the performance of the latent approach using fixed and projected tolerances for a case with an equivalence ratio of 0.9 and an initial temperature of 1440 K. When reducing the number of retained variables, q, *projected tolerances* achieve a reduction of computational time from the species transport case while using a similar number of steps. In contrast, *fixed tolerances* struggle to reduce computation time due to increased step counts, caused by mismatches in scale between the tolerances and the latent variables. Despite these differences, both approaches yield comparable accuracy, as indicated by similar R^2 scores.

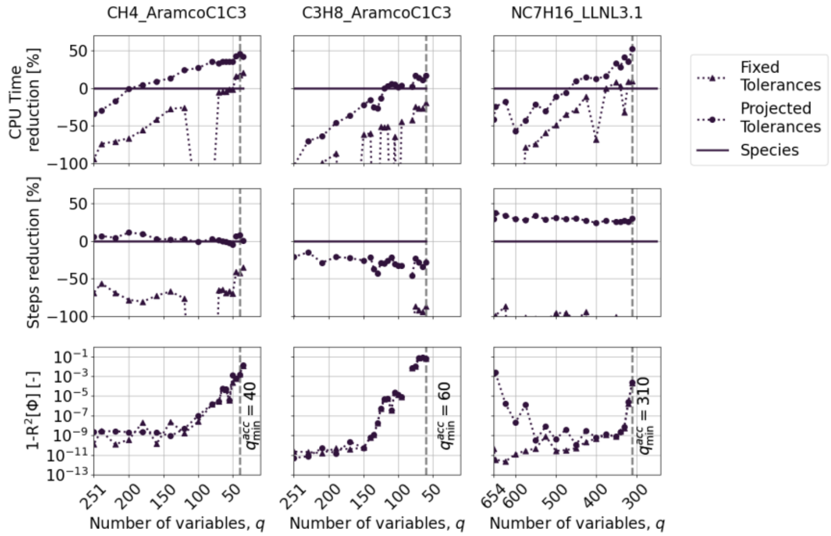

Figure 1. Computational performance and error committed by the latent solver with *fixed* and *projected tolerances*, compared with the species case, for a batch reactor with CH4, C3H8, and NC7H16 fuels at an equivalence ratio of 0.9 and an initial temperature of 1440 K.

Conclusions

This work presents an optimized latent variable transport method with direct computation of the source terms, achieving substantial computational savings compared to full-order simulations without compromising accuracy. Future work will focus on extending this approach to two-dimensional flame configurations.

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