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A co-kurtosis based dimensionality reduction for chemical kinetics using neural ODEs

Tadikonda Shiva Sai[1]*, Hemanth Kolla[2], Konduri Aditya[1]
*Lead presenter: shivast@iisc.ac.in
[1] Department of Computational and Data Sciences, Indian Institute of Science, Bengaluru, KA, India
[2] Sandia National Laboratories, Livermore, CA, United States of America

Reduced-order modeling (ROM) of reacting flows mitigates the high computational cost of detailed chemical kinetics in DNS and LES by projecting governing equations onto low-dimensional manifolds, with principal component analysis (PCA) being the most widely adopted technique for identifying variance-optimal modes. However, PCA considers second-order covariance, making it insensitive to rare, extreme-value events, such as ignition kernels, that exhibit non-Gaussian statistics. Co-kurtosis PCA (CoK-PCA) addresses this limitation by decomposing the fourth-order joint cumulant tensor to extract modes dominated by high kurtosis, thereby capturing the statistical signatures of such events better. *A priori* analysis demonstrated that CoK-PCA–based manifolds yield more accurate reconstructions of species concentrations and heat-release rates under aggressive truncation than standard PCA [1, 2].

In this study, we perform *a posteriori* analysis of the CoK-PCA-based ROM for auto-ignition in a homogeneous reactor. We evolve the reduced ODE system in the PC space using (i) a standard ODE solver with pre-trained neural network source term closures and (ii) an integrated neural ODE [3] solver that learns time integration during training. Our results show that the CoK-PCA manifold robustly reproduces ignition delay times and reaction-zone profiles, particularly heat release rates, and that the neural ODE approach further minimizes error accumulation over multiple steps. These findings highlight the potential of CoK-PCA-based manifolds and their coupling with neural ODE integration for embedding efficient and accurate chemistry in large-scale, parallel reacting-flow simulations.

References

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