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Predicting the evolution of chemical species using Neural ODEs[1]

PINAKI PAL, OPEOLUWA OWOYELE, Argonne National Laboratory — While running computational fluid dynamics simulations of combustion devices, one of the main bottlenecks remains the computation of the chemical species' source terms and integrating them. In recent years, deep learning-based methods have emerged as a promising approach to solve this problem, where artificial neural networks have been used to predict the source terms of chemical species as a function of the chemical state of the system. One main drawback of machine learning-based methods introduced in previous studies is that they minimize the *a priori* error (i.e., error during training), but do not guarantee that the errors during deployment in CFD will be small. In this work, we propose to address this issue by applying a recent class of neural networks, Neural ODEs, to learn to predict chemical source terms as functions of the current state. This approach is applied to the problem of a perfectly stirred reactor (PSR), and subsequently, to the simulation of a turbulent non-premixed flame in a mixing layer. It is shown that even when the dimensionality of the thermochemical manifold is trimmed to remove redundant species, the proposed approach accurately reproduces the results obtained with detailed chemical mechanisms, at a fraction of the computational cost.

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