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Accounting for variable time-steps in Neural Network accelerated kinetic computations.

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Abstract

The simulation of reactive flows presents significant challenges in various industrial sectors, including aeronautics and energy production. The coupling of fluid dynamics with chemistry is computationally expensive due to the wide range of spatial and temporal scales involved in chemical processes, resulting in stiff equations that require advanced numerical methods. Recently, machine learning has emerged as a promising approach for efficiently estimating reaction rates. In particular, Artificial Neural Networks (ANNs) are well-suited to this task, as they can perform high-dimensional data interpolation, making them particularly advantageous for complex chemistry problems. Such networks, trained on relevant databases, have been successfully applied in various combustion studies, ranging from non-premixed to premixed combustion and from steady cases to transient auto-ignition scenarios.

A critical aspect of applying ANNs is constructing an appropriate training database that is both representative of the target application and computationally efficient to generate. However, most databases only include the composition variations for a constant time-step, whereas many real-world applications require variable time-steps to be accurately described. This study addresses the challenge of training ANNs on databases with variable time-steps, proposing strategies to adapt the training process to these conditions. First, a method is introduced to generate variable time-steps databases from constant timestep databases. Then, the ability of different network architectures to learn from this database is evaluated. Finally, the implications of this approach for the broader applicability of ANNs in reactive flow simulations are discussed, highlighting the potential of this methodology to accommodate diverse combustion systems and dynamic conditions.

Keywords: Neural Networks, CFD, Chemical kinetic