OpenFOAM & Combustion Simulation

Machine learning-assisted modeling for combustion chemical models: Stiffness removal and model reduction

Prof. Tianhan Zhang

Southern University of Science and Technology, China

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Host: Prof. Wang Han (Beihang University)

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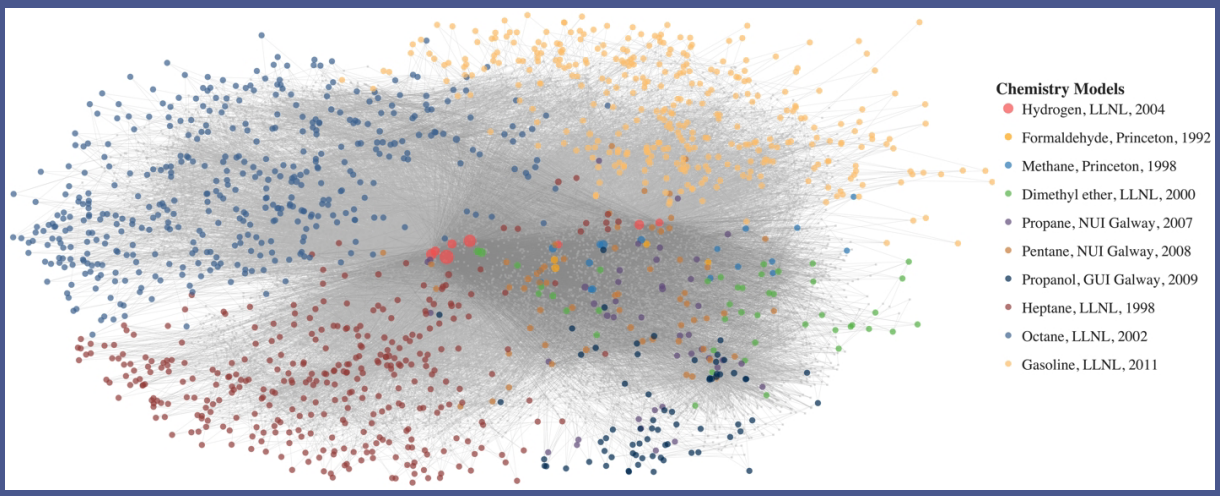
Abstract

Machine learning has been popular recently but has many limitations and drawbacks. This talk considers machine learning a powerful tool for fitting high-dimensional functions, which can be leveraged by combustion modeling to improve efficiency and generalization. The main focuses are on designing and training the target high-dimensional functions, given the complicated nature of the combustion data.

Two examples will be introduced in the talk. The first one is the DNN-based surrogate kinetic model to remove numerical stiffness. The results show that the DNN-based model covers auto-ignition to turbulent flame and reduces the computational cost of chemical kinetic calculation by one or two orders of magnitude. At the same time, the model has a plug-and-play feature for different kinds of CFD codes.

The second is a machine learning-based reinforced sampling method for model reduction. The current algorithm can reduce detailed mechanisms, such as LLNL n-heptane (648 species) or iso-octane (857 species) mechanisms, to a skeletal one with around 40 species, maintaining a satisfying accuracy on ignition delay time, laminar flame speed, and extinction limit at a wide range of conditions. The algorithm also shows an interesting discovery about the core sub-mechanism shared by C1-C8 reduced mechanisms.



About the Speaker

Dr. Tianhan Zhang is an assistant professor in the Department of Mechanics and Aerospace Engineering at Southern University of Science and Technology (SUSTech), China. After studying multiscale modeling from Professor Yiguang Ju and Professor Weinan E, he obtained his Ph.D. in Mechanical and Aerospace Engineering from Princeton University. He joined AI for Science Institute, Beijing in 2021 and SUSTech in 2022. His research focuses on numerical simulations with detailed combustion chemical models, including cool flame dynamics, detonation formation, and machine learning-assisted algorithms.