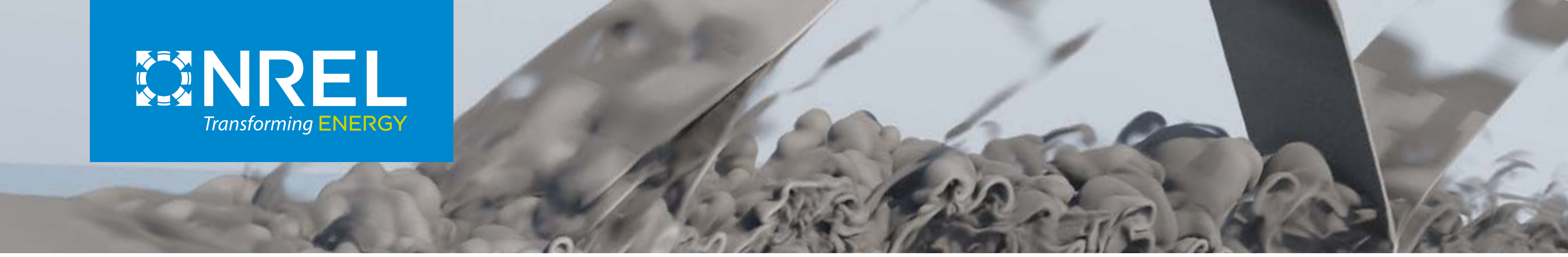
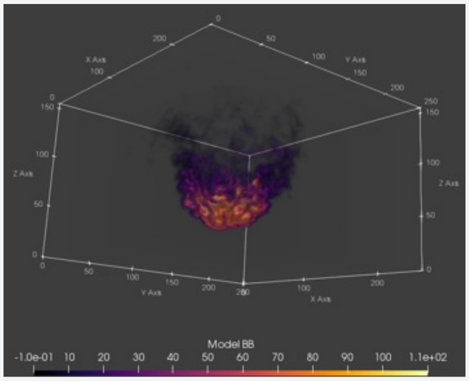


Visualization by Nicholas Brunhart-Lupo, NREL

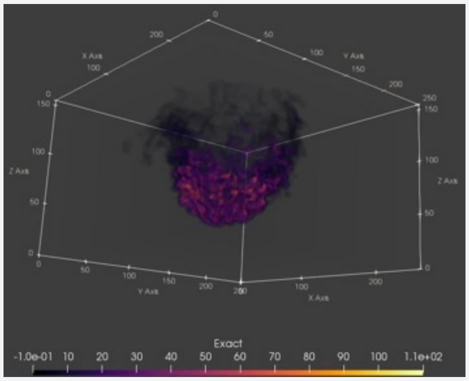
Transforming **ENERGY** through Computational Excellence

Exascale Computing: Combustion

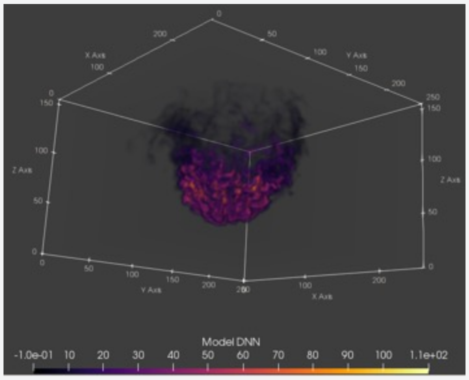
Deep Learning for Presumed Probability Density Function (PDF) Models



Analytical PDF model predicted reaction rates



Actual reaction rates



Deep learning PDF model predicted reaction rates

NREL researchers use advanced machine learning techniques to define improved methods using deep learning models to resolve reacting flows in turbulent combustion flows, reducing the computational burden, increasing computational speed, and improving accuracy. *These advancements reduce cost and improve fidelity of rapid-turn-around engineering calculations.*

Challenge

Leveraging exascale computing for simulation has the potential to accelerate the development of cost-effective combustion technologies. However, even with modern high-performance computing hardware, the computational cost and complicated nature of fully resolving reacting flows in these devices can be prohibitive.

Objective

The objective is to replace poorly performing common analytic models with deep learning models trained using high-fidelity calculations for the key components of subgrid physics. The purpose of these models is to better leverage computational resources for combustion simulation.

Approach

Researchers use three major classes of machine learning algorithms—traditional ensemble methods like random forests, deep neural networks (DNN), and deep generative unsupervised learning (conditional variable autoencoder)—to explore the accuracy of different PDF shape functionals for their use within a large eddy simulation model. Researchers judge the PDF shape functionals by their ability to reproduce the subgrid scales of a large-scale direct numerical simulation data set for specific reacting flow configurations.

Results

This study demonstrates that deep learning models for presumed PDF modeling are three times more accurate than commonly used analytical β–β (beta-beta) PDF models and linear regression models, and as accurate as random forest models while using five times fewer trainable parameters and being 25 times faster for inference.

This work—models, analysis scripts, Jupyter notebooks, and figures—can be publicly accessed at the project's GitHub page (https://github.com/NREL/ml-combustion-pdf-models).

Henry de Frahan, Marc T., Shashank Yellapantula, Ryan King, Marc S. Day, and Ray W. Grout. 2019. "Deep learning for presumed probability density function models." Combustion and Flame, Volume 208, 436-450, ISSN 0010-2180, https://doi.org/10.1016/j.combustflame.2019.07.015

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