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MACHINE-LEARNING TURBULENCE MODELS FOR SIMULATIONS OF TURBULENT COMBUSTION

Allocation: Strategic/75 Knh
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EXECUTIVE SUMMARY

Predictive simulations of turbulent combustion are crucial to the design of energy-conversion systems in the transportation, power, and defense sectors, among others. Due to their multiscale, multiphysics nature, these systems are typically intractable to simulation at full resolution. Lower-resolution simulations are possible but require closure models; currently, state-of-the-art closure models fail to capture key dynamics in certain regimes of turbulent combustion, and the use of these models can lead to incorrect predictions.

The research team has developed a novel approach for the design of turbulence closure models utilizing machine learning (ML) techniques and large-scale, fully resolved computational data sets. The team trains and refines neural network-based models across the problematic regimes, then refines the models using an adjoint solution, which is analogous to an on-the-fly error-control procedure. The resulting ML-based models are more accurate than the most commonly used models and can be generalized to different applications. Alternatively, the deep learning model can be harnessed to produce predictions of similar accuracy to those of existing models at reduced computational cost.

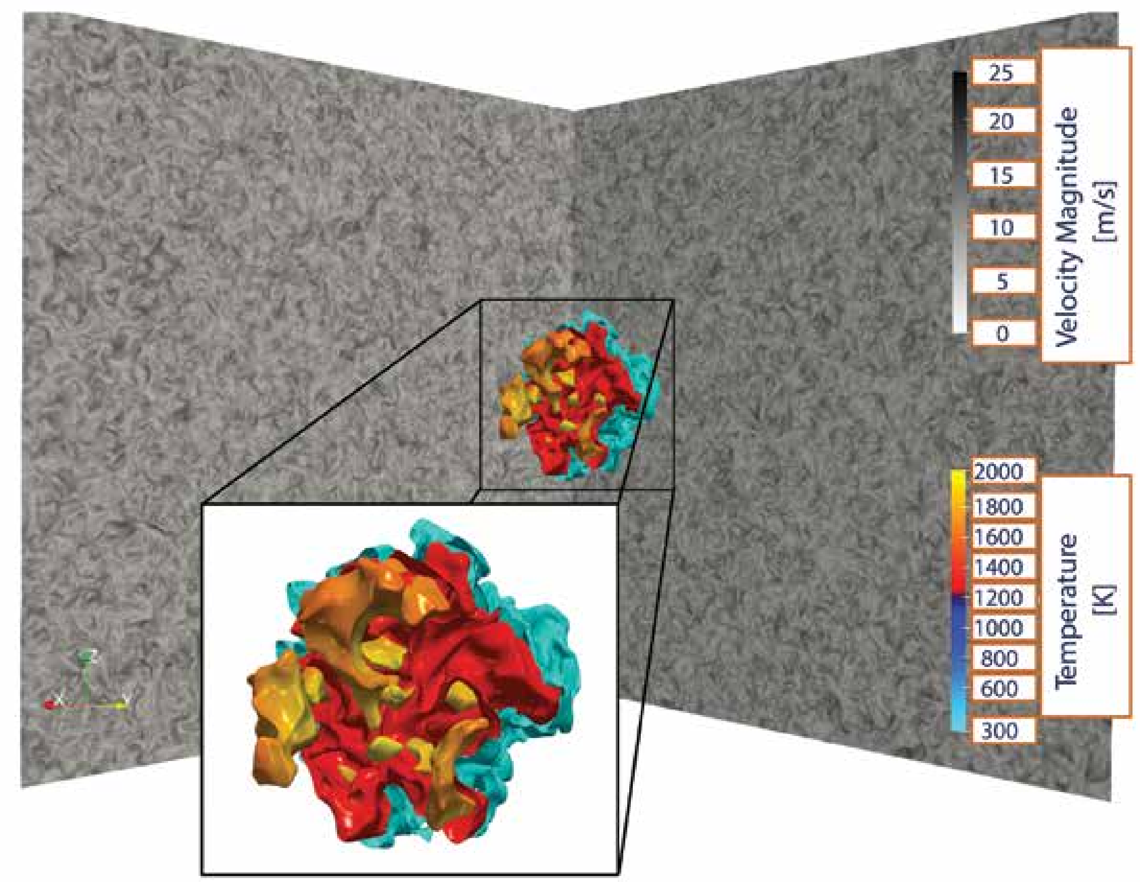

Figure 1: Illustration of a direct numerical simulation (DNS) of an expanding hydrogen–air premixed flame kernel (colored surfaces) in isotropic turbulence (grayscale background). The simulation is discretized using $1{,}024^3$ grid points and utilizes up to 16,384 cores. Machine learning models trained on many DNS databases are tested in analogous large-eddy simulations (LES).

RESEARCH CHALLENGE

Turbulent combustion is an inherently multiscale, multiphysics phenomenon relevant to virtually every sector in which chemical energy is converted to mechanical energy. Modern combustors for gas turbines, internal combustion engines, rocket propulsion, and hypersonic flight all require turbulent flow to enhance fuel–oxidizer mixing and to increase burning rates. Accurate prediction of the performance, efficiency, and emissions of these devices is an essential aspect of the engineering design and test cycle.

However, the most common closure models used to make these predictions computationally tractable are based on nonreacting turbulence theory and are known to fail in regimes relevant to the next generation of clean combustors. One key challenge is the prediction of turbulence–combustion interactions in premixed flames. These interactions are necessarily precluded by the use of nonreacting turbulence models [1–3]. Linearly coupled reacting-turbulence models have been developed [3,4] but are of limited use owing to their exclusion of nonlinear interactions. The research team therefore focuses on developing nonlinear models that are capable of capturing such interactions.

METHODS & CODES

The researchers have developed a machine learning approach to turbulence model development with a focus on predicting nonlinear turbulence–combustion interactions. Numerical databases from fully resolved direct numerical simulations (DNS) of turbulent combustion form the basis of these model-development efforts. The team generates DNS databases across a range of turbulent combustion regimes using the semi-implicit, second-order, energy-conservative code NGA [5,6]. These databases are subsequently downsampled using a low-pass filter to obtain flow fields comparable to those obtained from a large-eddy simulation (LES; *i.e.*, modeled) calculation. Because the filtered fields originate from full-resolution data, the "true" model outputs are also available. Using deep neural networks as a nonlinear statistical model, the team approximates these "true" outputs from input variables that are available in LES. The resulting models are tested *a priori* using out-of-sample DNS data and *a posteriori* by implementation in analogous LES calculations. As a novel approach to model development, they have developed a new DNS/LES code, PyFlow, that is capable of refining the model during the *a posteriori* step using an adjoint solution. This code is GPU-accelerated and has potential to address modeling challenges over a wide range of flows.

RESULTS & IMPACT

The initial results show an encouraging ability of the machine learning-based models to predict turbulence–combustion interactions more accurately than traditional turbulence models. These findings are obtained from *a priori* testing and demonstrate that ML-based models have the potential to supplant traditional turbulence models in LES. However, in *a posteriori* testing, the researchers found that numerical errors (including finite-difference errors) owing to the reduced LES resolution accumulate in neural network inputs and reduce the models' predictive accuracy. The issue of numerical error is unavoidable in LES but can potentially be mitigated using the team's *a posteriori* model refinement step. By training *in situ*, models can be developed that are less sensitive to numerical error, for example, by reducing weights associated with error-prone inputs and hidden parameters. The *a posteriori* training step, therefore, represents a potentially significant contribution to ML-based model development and LES of turbulent combustion.

WHY BLUE WATERS

This research relies on both CPU-only and GPU-accelerated compute nodes for different tasks. Because Blue Waters offers both types of nodes on a common file system, data access and sharing are greatly streamlined among tasks and project members. Additionally, the team utilizes Blue Waters-specific Python installations and packages that are supported by NCSA project staff. These installations are optimized for Blue Waters and offer substantially improved application performance compared to user-installed libraries.