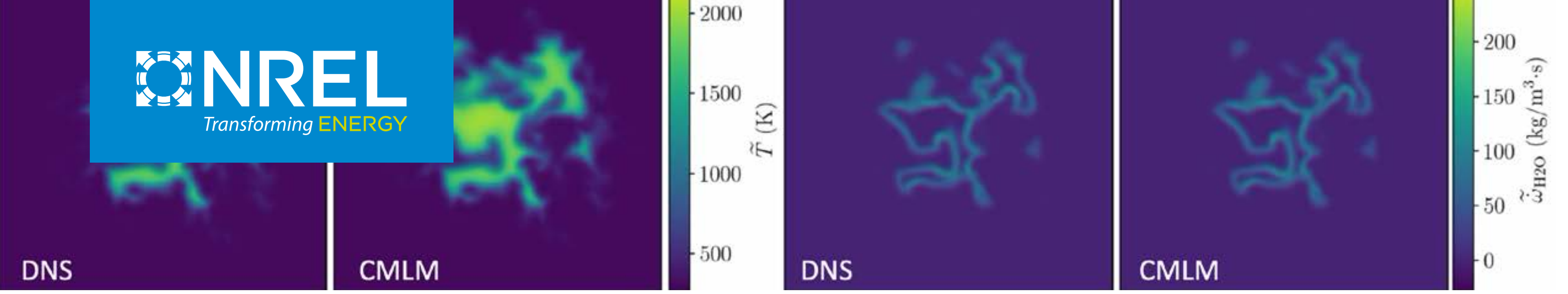

Transforming **ENERGY** Through Computational Excellence

Co-Optimized Machine-Learned Manifold Models for Large Eddy Simulation of Turbulent Combustion

Challenge: Simulation of turbulent combustion is imperative to enable the development of low carbon combustion-based energy conversion technologies that operate in novel regimes. However, simulations are also *challenging and computationally demanding* because of the *complex chemical mechanisms* that describe the conversion of fuel and oxidizer to products and the *wide range of length scales* of the important chemical and turbulent flow processes. A major objective of turbulent combustion research is to overcome these challenges through modeling approaches that provide computationally affordable but still sufficiently accurate predictions.

Approach: The co-optimized machine-learned manifolds (CMLM) approach is a data-driven method of generating manifold-based models for turbulent combustion that combines *dimension reduction, calculation of reaction rates and other thermochemical quantities*, and, optionally, *subfilter closure for Large Eddy Simulation (LES)* into the structure of a *single neural network*, shown in Fig. 1. This method allows the optimization algorithm used to train this network to simultaneously optimize all three elements, leading to better overall performance than when they are considered separately. The CMLM network is designed to yield manifold variables that are sparse linear combinations of species, allowing for interpretability and simpler transport equations that are analogous to those used for flamelet- and Principal Component Analysis-based models. The method can be applied with any set of training data, making it very flexible. It has now been incorporated into the Pele suite of combustion simulation codes to allow for assessment of model performance when coupled into real combustion simulations.

Results: CMLM has been demonstrated using a priori (stand-alone) tests based on data from one-dimensional premixed flames and Direct Numerical Simulations (DNS) studies of turbulent premixed ignition kernels. In the simpler case, it produces a model similar to the flamelet-generated manifolds (FGM), but with slightly better performance, demonstrating

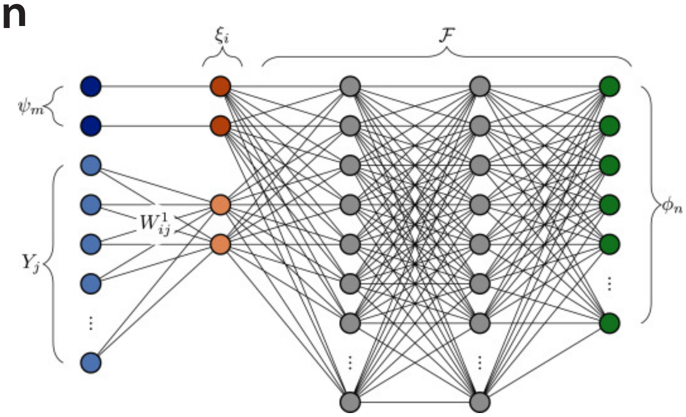

Fig. 1. Structure of the neural network that combines the definition of manifold variables (shades of orange) from species mass fractions (blue), other inputs (dark blue), and the nonlinear mapping F to the model outputs (green) into a unified manifold discovery process. *Image from B.A. Perry, M.T. Henry de Frahan, S. Yellapantula. Combustion and Flame 244C (2022) 112286 https://doi.org/10.1016/j.combustflame.2022.112286*

the ability of the data-based approach to recover known physics. But CMLM can efficiently incorporate data from more-complex simulations, *allowing it to extend beyond the limits of physics-based models*. CMLM can reduce the cost or further improve accuracy of existing approaches that have already shown promise across many combustion modeling studies.

Impact: CMLM is dramatically more efficient than solving equations for all species involved in combustion, while also maintaining accuracy. The number of scalar equations that are solved has been reduced from 30 to 2, and the cost of simulation is reduced by an order of magnitude. This progress, using CMLM and other manifold models, will enable the Pele codes to be applied for engineering simulations to optimize key energy systems, such as aviation combustors that burn sustainable aviation fuel. Particularly, CMLM can leverage the large data sets generated by using the Pele codes for detailed scientific simulations to generate models then used in simulations that assess parametric and design sensitivities.

Top: Initial simulations show predictions that are quite similar to those using detailed chemistry, for example for predicting the ignition of jet fuel. *Image from B.A. Perry, M.T. Henry de Frahan, S. Yellapantula. Combustion and Flame 244C (2022) 112286 https://doi.org/10.1016/j.combustflame.2022.112286*

National Renewable Energy Laboratory
15013 Denver West Parkway, Golden, CO 80401
303-275-3000 • www.nrel.gov

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