Adaptive Depth Neural Networks for Scale-Bridging Modeling of Multiphase Reacting Flows

The goals of this research project were to address challenges and provide an automated, efficient framework for data-based modeling. To address these challenges, new approaches were developed for multiple data-based modeling components, including data pre-processing containing outlier removal and data sampling; input dimensionality reduction using principal component analysis and a new concept of dimensional consistency of input and output; and modeling, including efficient regression and automatic deep neural networks architecture/hyperparameter optimization using Bayesian Optimization and a quick adaptive-depth neural network approach. This data-based modeling framework was ultimately used to develop a model for the filtered drag in coarse-grained simulations of multiphase flows.
### Accomplishments:
In this project, an efficient, automated data-based modeling framework was developed and applied to key modeling challenges in reacting and multiphase flow. The data-based modeling framework relied on three components including data pre-processing, input dimensionality reduction, and modeling (i.e., regression). Two automated procedures were developed: the Bayesian Optimization approach requires more training time but results in a more compact network while the Adaptive Depth Neural Networks approach requires less training time but results in a larger, more complex network. The data-based modeling framework was applied to key modeling challenges in both reacting flows and multiphase flows. For reacting flows, the framework was used to develop non-universal scalar dissipation rate profiles, which are key inputs to manifold-based turbulent combustion models. For multiphase flows, the framework was used to develop and better understand the filtered interphase particle drag. Additionally, the framework was used on a NETL dataset to showcase its capabilities.

### NETL Collaboration:
The data-based modeling framework developed as part of this work was leveraged to analyze datasets under investigation by NETL. In parallel with this research project, NETL has been developing the capabilities to include data-based models in MFiX. Through the project, NETL provided datasets to test with this framework, ending with a full dataset which included 170,000 samples.

### Relevant Publications:


### Benefits:
Overall, the framework is truly automated and requires no user intervention and input. From this perspective, this framework achieves the ultimate goal of data-based modeling: data equals model. Data-based modeling is a critical need in all application domains. While the framework developed in this project was applied to reacting and multiphase flows, the automated framework is agnostic to the application domain. This opens endless possibilities to applying the framework in any context to develop data-based models.