University of Stuttgart
Institute for Combustion Technology (ITV)

Bachelor or Master Thesis

Towards the Application of Machine Learning in Sooting Flames

Motivation

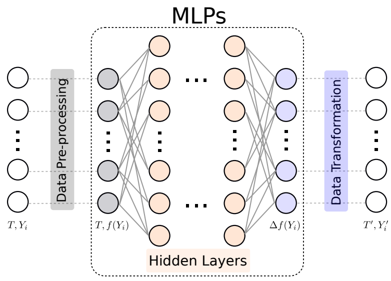
Reliable simulations pertaining to soot remain a considerable challenge. One of the primary reasons for this challenge is the intricate nature of fuel/soot mechanisms, which can consist of hundreds of species. Direct integration (DI) of the extensive and stiff ordinary differential equations (ODEs) accounts for over 90% of the total CPU hours, thereby limiting the feasibility of high-fidelity soot simulations. Artificial neural networks (ANNs) are a powerful tool for emulating non-linear systems. They are universal function approximators and have both the advantages of high mapping complexity and high computational speed. Therefore, utilizing ANN techniques for modeling thermodynamic evolution in sooting flames holds great promise.

Project description and research goals

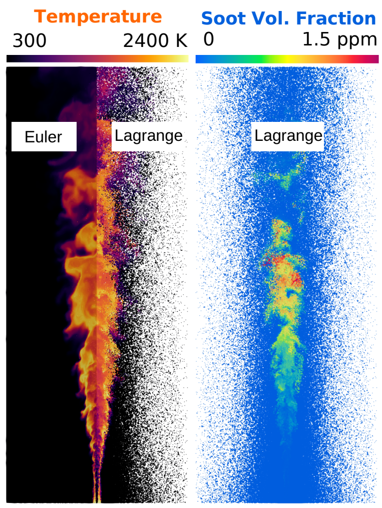
As ANN models are data-driven, a good preparation of training datasets is a pivotal factor in determining the model performance. A dataset with scarce samples results in a rigid model as predictions become unforeseeable when confronted with data points outside the training space. Nevertheless, dealing with a larger dataset doesn't guarantee success either because (1) reaching a satisfying loss error is then arduous and time-consuming, and (2) the sample distribution within the dataset is believed to have a greater importance. Besides, recent studies have shown that splitting the composition space, especially for high-dimensional spaces, is a critical step to obtain reliable ANN models. This project aims to delve into the influence of sample distribution on model performance. Moreover, two splitting methods will be compared and analyzed.

Tasks

- Do a literature review to learn about the ideas of using machine learning to approximate thermodynamic evolution
- Train a ANN model using a eight-species hydrogen mechanism and analyze how does the sample distribution affect model performance
- Compare K-means clustering and species grouping methods for composition space decompositions
- Implement sampling and space splitting strategies to ethylene flames using the UCS mechanism (with 32 species)
- Write a thesis and present your results



(a) An illustration of the ANN structure.



(b) Instantaneous fields of temperature and soot volume fraction in the Sandia flame.

Prerequisites

- Basic knowledge in machine learning and reacting systems, programming with Python or similar
- Beneficial: knowledge in pyTorch and C/C++, experience with computational fluid dynamics (CFD), OpenFOAM

Contact

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