Research on Machine Learning Algorithms for Modeling Large Eddy Simulation Closures of Reacting Flows

MSc Thesis Proposal

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The aim of this master's thesis research project is to develop a data-driven Machine Learning (ML) framework for the modeling of closure terms in Large Eddy Simulations (LES) of hydrogen reacting flows.

LES is a very efficient method for computing turbulent flows in practical applications. It consists of filtering and modeling small-scale flow physics that would otherwise be very computationally expensive to resolve. However, modeling physics at the subfilter-scale level can be extremely challenging, especially when numerous physical phenomena interact. Computational physicists have been working hard to address this issue, deriving analytical laws to model subfilter features. Recently, ML has been proposed as an alternative in this field [1]. ML algorithms enable to approximate non-linear mapping from resolved to subfilter quantities (closure terms) without a priori modeling assumptions. They are therefore particularly powerful when the underlying physical phenomena are poorly understood and conventional analytical closures fail. This project aims to further develop ML methods with an application to the modeling of subfilter-scale hydrogen turbulence-chemistry interactions. It is a significant challenge due to differential diffusion that causes thermodiffusive instabilities and strong variations of the reaction rates along the flame fronts when the H_2-air mixture is lean and premixed [2].

The idea is to continue the work of Ref. [3] by training the model to infer all the closure terms of the multi-species, reacting Navier-Stokes equations. We will start by generating a database of hydrogen flames with a simple one-step chemistry. Then, explicit filtering and downsampling will be performed to emulate LES solutions. Supervised Learning (SL) will be employed to train a CNN to infer the closures on this database. If time allows, we will eventually implement the CNN model in an LES solver for online inferences.

This interdisciplinary project brings together reacting flows, computational sciences and machine learning. It is very important for the development of computing models for the combustion of H_2, a carbon-free fuel that could lead to more sustainable power systems. Experience with HPC code development would be greatly beneficial to this project.

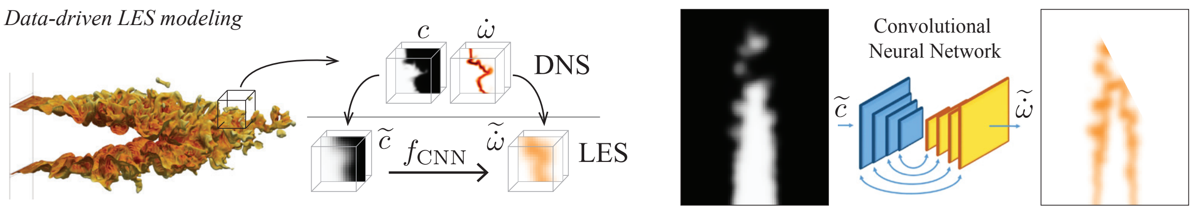

Figure 1: Diagram of training strategy on filtered DNS field and inference on solution field. From [3].

References

[1] R. Vinuesa and S. L. Brunton, "Enhancing Computational Fluid Dynamics with Machine Learning," *Nature Computational Science*, vol. 2, pp. 358–366, June 2022.

[2] H. Pitsch, "The transition to sustainable combustion: Hydrogen- and carbon-based future fuels and methods for dealing with their challenges," *Proceedings of the Combustion Institute*, vol. 40, no. 1-4, p. 105638, 2024.

[3] Q. Malé, C. J. Lapeyre, and N. Noiray, "Hydrogen reaction rate modeling based on convolutional neural network for large eddy simulation," *Submitted to Data-Centric Engineering, arXiv:2408.16709 [cs.CE]*, 2024.