Research on Deep Reinforcement Learning for Modeling Subgrid-Scale Wrinkling of Reaction Fronts in Large Eddy Simulations

MSc Thesis Proposal

Harvard John A. Paulson School Of Engineering And Applied Sciences
Computational Science & Engineering Laboratory
Contact: Quentin Malé, qumale@ethz.ch

The aim of this master's thesis is to develop Deep Reinforcement Learning (DRL) methods for modeling SubGrid-Scale (SGS) flame wrinkling of thickened flames in Large Eddy Simulations (LES). The artificial thickening of flame fronts is a powerful strategy allowing for the resolution of the flame front on LES computational grids [1, 2]. Following simple theories of laminar premixed flames, the flame speed S_L and the flame thickness δ_L may be expressed as

$$S_L \propto \sqrt{D_{th} B} \ \text{ and } \ \delta_L \propto \sqrt{D_{th}/B}\,. \tag{1}$$

where D_{th} is the thermal diffusivity and B the pre-exponential constant. If D_{th} is increased by a factor F while B is decreased by F, the flame thickness δ_L is multiplied by F while the flame speed is maintained. It is therefore possible to thicken reaction fronts while maintaining their correct propagation speeds. The thickening factor F can be adjusted so that the thickened flame front is sufficiently resolved on the grid. However, when the ratio between the turbulence length scale and the laminar flame thickness is decreased, the flame becomes less sensitive to turbulence motions (Fig. 1). An efficiency function E corresponding to a SGS wrinkling factor needs to be derived to account for the loss in flame wrinkling due to thickening. Many analytical laws have been derived to model the wrinkling factor E (e.g. [1, 3]) and this method has proved highly successful. However, wrinkling is assumed to be due to turbulence only, and this does not take into account wrinkling due to thermodiffusive instabilities, for example. This is a current problem for the development of Hydrogen (H_2) combustion systems, where the molecular diffusion of H_2, much faster than heat, causes substantial additional wrinkling. The interaction between turbulence and thermodiffusive effects is not well understood, motivating a Machine Learning (ML) approach to model H_2 flame propagation in LES.

The idea is to train a ML model based on DRL to approximate the efficiency function E to retrieve the correct turbulent flame propagation from a Direct Numerical Simulation (DNS) surrogate. We will start with a simple 2D case with one-step chemistry and no preferential diffusion to model only the SGS flame wrinkling due to turbulence. We will need to set up a framework for training DRL agents with repeated LES realizations. As the project progresses, thermodiffusive effects may be introduced to assess the method's ability to take SGS thermodiffusive instabilities into account. Eventually, we will be able to move on to more realistic 3D cases.

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.

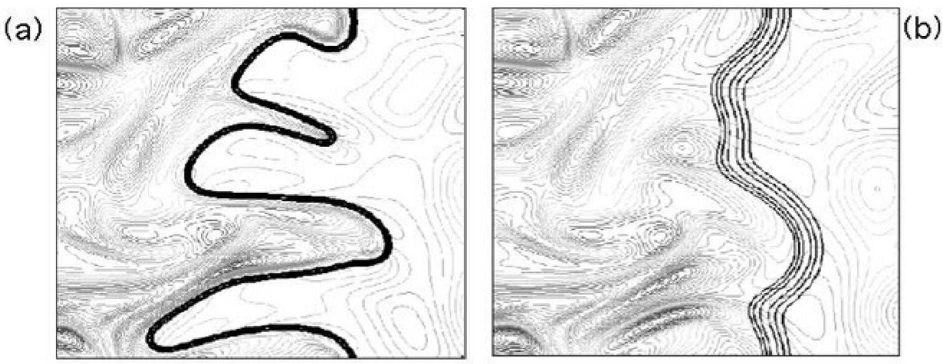

Figure 1: DNS of flame turbulence interactions. (a) reference; (b) artificially thickened flame with $F = 5$. The thickened flame is less wrinkled by turbulence motions. From [2].

References

[1] O. Colin, F. Ducros, D. Veynante, and T. Poinsot, "A thickened flame model for large eddy simulations of turbulent premixed combustion," *Physics of Fluids*, vol. 12, pp. 1843–1863, July 2000.

[2] T. Poinsot and D. Veynante, *Theoretical and numerical combustion.* Toulouse: CNRS, 3. ed ed., 2011.

[3] F. Charlette, C. Meneveau, and D. Veynante, "A power-law flame wrinkling model for LES of premixed turbulent combustion Part I: non-dynamic formulation and initial tests," *Combustion and Flame*, vol. 131, pp. 159–180, Oct. 2002.