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Machine Learning Accelerated Computational Multiphysics

Efficient simulation of physicochemical processes is central for engineering design. These processes typically consist of multiphase flow, heat and mass transfer, reaction and transport of chemical species in multicomponent mixtures, and turbulence. These complex processes span a wide range of space and time scales, making experimentation inefficient and often infeasible for preliminary design. Simulations present a safe alternative to physical prototyping and testing while providing engineers with detailed insights of the system of interest, allowing superior designs at low risk and cost. This is accomplished with high-throughput design screening, which requires the simulation of a class of systems in a regime with only small variations to the geometry or fluid parameters. Thus, it is important for simulations to run quickly so that many configurations can be tested efficiently. Numerical solutions should be accelerated by leveraging past iterations of simulations under similar conditions. This can be accomplished with Machine Learning techniques.

Machine learning (ML) has shown promising results in many computational fluid dynamics applications such as turbulence closure modelling, operator learning, and ML-accelerated physics solvers. This work is focused on the branch of ML-accelerated computational multiphysics, which seeks to combine classical numerical methods with data-driven deep learning techniques to accelerate simulations. Despite rapid progress, current work in this field lacks key features required to be used effectively in practice by engineers. This work aims to bridge that gap by incorporating engineering expertise into the design process. Specifically, an automated framework combining traditional multiphysics software and ML methods is developed and validated for 2D steady flow problems.