Title: Small closure models for large multiscale problems

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Project description

Mathematical modelling of multiscale phenomena is an important and challenging area of research, with applications including weather and climate predictions, energy generation and the discovery of new materials. Since these problems contain a wide range of spatio-temporal scales that cannot all be solved directly on a computer, the governing equations that describe these phenomena need to be simplified. This simplification often leads to Partial Differential Equations (PDEs) with an unknown (i.e. unclosed) source term, for which a suitable model must be found. Despite decades of research, these closure models remain highly empirical, and their shortcomings can significantly corrupt the predictions.

In recent years, Machine-Learning (ML) approaches have therefore been used to learn new closure models from data. Often, the uncertainty of a multiscale system lies mainly with the unknown closure term, which is part of a wider PDE system that is otherwise known. It therefore makes sense to not completely 'relearn the wheel', and only apply ML at the source of uncertainty, i.e. by replacing only the closure term with a ML model, rather than learning an entire system which is already partially known. Two important challenges in such coupled PDE-ML systems are:

1. Even in the simplified governing equations, the spatially-extended closure terms can easily have millions of degrees of freedom. This can result in memory constraints, and requires us to learn the very complex spatio-temporal structure of the closure term.

2. Traditional ML training is not geared towards coupled PDE-ML systems, and can result in biased (or even unstable) results, due to error accumulation in the PDE-ML interaction.

We have developed a new dimension reduction methodology (see [1]) to tackle the first challenge, thus far applied a 2D turbulent flow model. This significantly reduces the amount of information that must be learned from data. Potential Msc projects can include:

- Extend the dimension-reduction method to three-dimensional problems in turbulence. This has the potential of far greater dimension reduction.
- Directly learn the full closure term using convolutional neural networks for 2D flow problems, without dimension reduction.
- Use recurrent neural networks (or some other ML method suited for time series) to learn the small remaining unclosed components from the dimension-reduction method, and study the stability of the coupled PDE+ML system.

References:

[1] Edeling, W., & Crommelin, D. (2020). Reducing data-driven dynamical subgrid scale models by physical constraints. Computers & Fluids, 201, 104470.