

## **Machine learning for stochastic parameterization and closure modeling in multiscale systems**

For numerical simulations of multiscale systems, modeled with differential equations (PDEs or ODEs), often it is computationally too expensive to resolve all relevant degrees of freedom in the computational model. To make simulations feasible, only part of the system is explicitly resolved, and the effect of the unresolved part is represented in a simplified way through a so-called parameterization or closure. Typically, it is the large-scale (macroscopic) part of the system that is explicitly resolved, and the small scales are parameterized. This fundamental challenge of parameterizing unresolved scales is encountered in many domains, ranging from climate modeling to computational chemistry.

Deriving parameterizations from first principles is often infeasible, and an emerging alternative is to use data-driven methods to construct parameterizations. In this project the aim is to employ machine learning (ML) techniques for data-driven parameterization. More specifically, the intention is to construct ML-based parameterizations that are inherently stochastic, using ML techniques for generative modeling. Some open research questions are how to train such an ML-based parameterization, and how to ensure good performance and stability of the hybrid computational model (consisting of the ML-based parameterization coupled to the discretized PDE). Several prototype models are available as testbed, stemming from atmospheric science, fluid dynamics and molecular dynamics.

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