ML-enhanced Numerics: From Super-resolution to Neural Operators for Parallel-in-Time Methods

Many models in computational science and engineering are based on time-dependent partial differential equations, e.g., the Navier-Stokes equations governing fluid dynamics. Hence, integration along the time axis arises as an important numerical problem in many domains. While spatial domain decomposition is a well-established parallelization strategy, on its own it will not suffice to provide the massive degree of concurrency required by upcoming exascale systems. Parallel-in-time (PinT) methods provide additional concurrency along the temporal axis and can improve parallel scaling. Classical PinT methods like Parareal rely on a computationally cheap coarse integrator to propagate information forward in time, while a parallelizable expensive fine propagator provides accuracy. Typically, the coarse method is a numerical integrator using lower resolution, reduced order or a simplified model. Recent progress on how to solve differential equations with techniques from machine learning can offer an alternative approach to hand-crafted numerical coarse models.

In this talk, we first explore how super-resolution techniques can enhance low-resolution numerical simulations in the ICON-O ocean model. Our method augments a coarse, mesh-based algorithm with frequent, learned corrections that incorporate the effects of unresolved dynamics, resulting in an effectively submesoscale-resolving simulation.

In the second part, we examine how physics-informed neural operators (PINOs) can improve parallel-in-time methods like Parareal and parallel spectral deferred correction methods (pSDC). We demonstrate that PINO-Parareal converges as fast as a bespoke numerical coarse model but provides better overall speedup than space-time parallelization with a numerical coarse propagator. Using Rayleigh-Bénard convection as a case study, we then show how pSDC can improve scaling, and discuss limitations of applying neural operators in this context.