Machine learning based coarse propagators for Parareal

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Parallel-across-the-steps methods like Parareal or MGRIT require the user to define one or multiple coarse level models. Achievable performance is very sensitive to how these models are constructed: they typically run with serial dependencies and thus limit speedup according to Amdahl's law, therefore they need to be fast to compute. However, their accuracy determines the number of iterations required for convergence so they must still be reasonably accurate. Finding good coarse models can be a complicated, laborious process and good solutions depend heavily on the specific problem.

In recent years, machine learning techniques for solving differential equations have reached some level of maturity. Physics-informed variants like physics-informed neural networks (PINNs) or physics-informed neural operators (PINOs) use the residual of a differential equation in the loss function to "teach" the network the physics of the solved problem. While these approaches tend to be less accurate than numerical solvers, they are fast to evaluate once trained and also fairly generic - at least in theory, all that is required to solve a different problem is modifiying the loss function, although in practice a small (or not so small) amount of hyperparameter tuning might be necessary.

ML-based methods are promising as coarse models in PinT. They are fast (at least as long as training times can be ignored), reasonably accurate and generic in the sense that they can be adopted to different problems by changing the loss function. In contrast to mesh-based numerical algorithms, they also easily deliver good GPU performance. Combinations of ML and numerical methods via PinT could therefore improve utilization of heterogeneous high-performance computing systems. And lastly, using ML in PinT could allow to tell when the network moves into untrained regimes - in contrast to a pure ML approach, which will simply deliver a wrong solution, a deterioration in accuracy of the ML model because parameters are too far away from the training data should show up in increasingly bad convergence of the PinT method.

The talk will present our attempts to build coarse models for Parareal using a modified PINNs or a PINO approach. Performance results will be shown for the one- and two-dimensional Black-Scholes equation. In some cases, the much cheaper coarse model delivered by ML can produce significant improvement in speedup from Parareal compared to a numerical coarse propagator.