Combining numerical methods and machine learning

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Almost all areas in the physical or engineering sciences rely on computational models to some extent. These models can be based on fundamental physics processes (physics-based) which typically leads to a set of differential equations. Alternatively, machine learning techniques can be used to infer input-output relations out of very large sets of data. Both approaches come with different strengths and weaknesses but they rely on mathematical algorithms to function reliably and efficiently. In the last couple of years, we are also increasingly seeing synergies between both worlds, for example when ML is used as part of a numerical algorithm for solving the differential equations of a physics-based model [1].

Our poster will present three case studies for combining ML and numerical methods. The first one will be a demonstration how a physics-informed neural network (PINN) can be used to build efficient coarse propgators for the parallel-in-time method Parareal [2]. Parareal parallelizes integration of initial value problems by iterating between a parallel fine solver and a serial coarse propagator. Since the coarse method constitutes a serial bottleneck, it needs to be computationally cheap but still accurate enough to ensure fast convergence.

The second case involves computation of trajectories of inertial particles in a fluid. Their movement is governed by the Maxey-Riley equations [3], but since this is an integro-differential equation, it is difficult to solve numerically. We will show some results attempting to train a long short-term memory (LSTM) network from numerical data to reproduce trajectories.

Lastly, we show results for a PINN attempting to identify the velocity and diffusion parameters in an advection-diffusion problem from synthetically generated tracer data.

References

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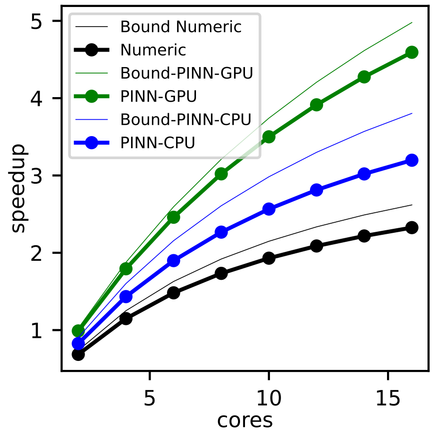
[3] Maxey, M. R. and Riley, J. J. 1983. Equation of motion for a small rigid sphere in a nonuniform flow. *The Physics of Fluids* 26:4.



Source: [2]

Figure 1: Parallel speedup of a Parareal parallel-in-time algorithm based using only numerical algorithms (black) versus a combination of numerical and ML techniques (green and blue). Combining onumerical with ML-based techniques significantly improves performance. Furthermore, integrating a ML-component helps to utilize GPUs more efficiently.

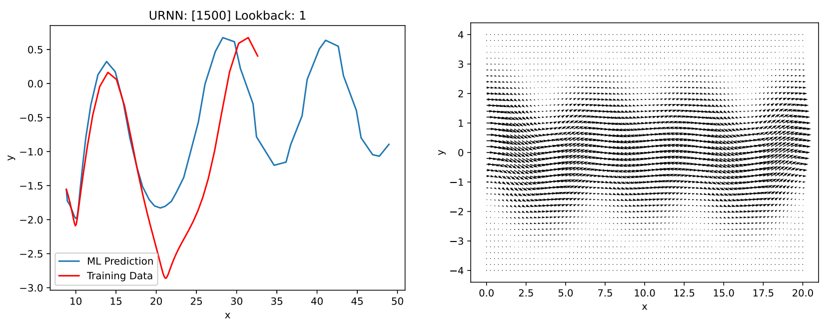


Figure 2: Trajectories of a particle (left) computed with a numerical solver (red line) and a LSTM neural network (blue line). The particle moves in a Bickley jet velocity field (right).

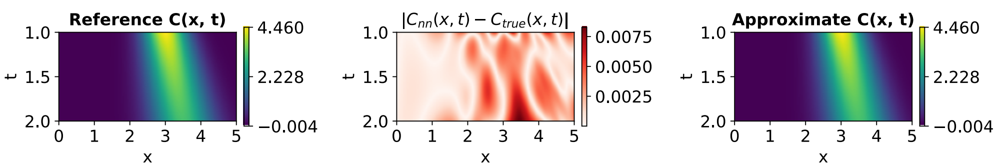


Figure 3: Reconstruction of the concentration of a tracer from synthetically generated data using a physics-informed neural network (PINN). Shown is the ground truth (left), the absolute error (midde), and the reconstruction from the PINN (right).