Contribution ID: **19** Type: **Spotlight talk**

Large-Scale Neural Solver for partial differential equations

Monday 6 December 2021 13:00 (15 minutes)

Solving partial differential equations (PDE) is an indispensable part of many branches of natural science. The analysis of experimental data by numerical simulation typically requires costly optimisation or grid-scan which is very costly. Machine Learning based surrogate models denote promising ways for fast approximation of these simulations by learning complex mapping from parameters to solution. However, recent surrogate models require a considerable amount of training data derived from full simulation runs, introducing a high storage demand as well as computational complexity especially if high-dimensional high-fidelity simulations are considered. Physics-informed neural networks denote a mesh-free approach which rely only on data for initial/boundary conditions. However, the most recent implementations of PINNs are not suited for high-fidelity problems because there is no multi-gpu implementation available making them intractable for scientific applications at FWK. We, the Helmholtz AI YIG at FWK, developed a library called Neural Solvers enabling large-scale distributed training of Physics-informed Neural Networks. We primarily aim at solving forward and inverse problems in Laser- as well as Plasma Physics such as 3D laser propagation for advanced understanding of Laser-plasma accelerators with very low storage footprint while retaining physical correctness of the trained surrogate model. The framework is ready for cross-disciplinary applications such as atom physics for simulation and inversion of density functional theory, geophysical inversion of acoustic wave equation, as well as inversion of 2d heat equation based on experimental neuroimaging data. Our experiments have shown that Neural Solvers can reach the accuracy of recent numerical methods while introducing excellent speedup up to at least 180 NVIDIA V100 GPUs making them ready for upcoming exascale systems. In the future, we will be researching parameterized PINNs to learn the solution of a set of simulations concurrently while transfer learning will be used to transfer knowledge from data of lower fidelity to high-fidelity problems.

Physical Presentation

I am not so sure at this point if I would present physically.

Primary authors: Mr STILLER, Patrick (Helmholtz-Zentrum Dresden-Rossendorf); Mr BETHKE, Friedrich (Helmholtz-Zentrum Dresden-Rossendorf); Mr ZHDANOV, Maksim (Helmholtz-Zentrum Dresden-Rossendorf); Mr RUSTAMOV, Jeyhun (Helmholtz-Zentrum Dresden-Rossendorf)

Co-authors: Mr BÖHME, Maximilian (Center for Advanced Systems Understanding); Mr EMAM, Ahmed (Helmholtz-Zentrum Dresden-Rossendorf); Dr HENDRIK, Paasche (Department Monitoring- und Erkundungstechnologien,Helmholtz-Zentrum für Umweltforschung - UFZ); Mrs MÜLLER, Juliane (Faculty of Medicine Carl Gustav Carus Clinical Sensoring and Monitoring); Prof. KOCH, Edmund (Technische Universität Dresden Faculty of Medicine Carl Gustav Carus Clinical Sensoring and Monitoring); Dr PAUSCH, Richard (Helmholtz-Zentrum Dresden-Rossendorf); Dr DEBUS, Alexander (Helmholtz-Zentrum Dresden-Rossendorf); Dr CANGI, Attila (Center for Advanced Systems Understanding, HZDR); Dr BUSSMANN, Michael (Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf); Dr HOFFMANN, Nico (HZDR)

Presenter: Mr STILLER, Patrick (Helmholtz-Zentrum Dresden-Rossendorf)

Session Classification: Parallel Session