Les Houches Summer School 2022 Application

The intersection of physics and machine learning has been the focus of my graduate career and undergraduate training. I am a PhD candidate in the Matter Under Extreme Conditions group at the Center for Advanced Systems Understanding (CASUS), Helmholtz-Zentrum Dresden-Rossendorf (HZDR) in Görlitz, Germany, under the supervision of Dr. Attila Cangi.

I work on accelerating quantum dynamics simulations through machine learning. My research goal is to develop Density Functional Theory (DFT) based simulation frameworks for electron dynamics for matter under extreme conditions. Specifically, I am developing machine learning accelerated solvers for Kohn-Sham equations, which are high-dimensional non-linear PDEs, in the time-independent [1] and time-dependent [2] domains. I am currently pursuing two lines of inquiry that are relevant to the summer school curriculum:

1. Physics Informed Neural Networks (PINNs) [3; 4]: Incorporate constraints posed by differential equations, including boundary and initial conditions, into the loss function of machine learning algorithms. Mesh-free nature is suitable for high dimensional PDEs with arbitrary resolution.
   - Challenge: Design and parametrization of the loss function to enforce constraints such as normalization and uniqueness of solutions. I am also exploring time-dependent regularization schemes for dynamical systems.

2. Graph Neural Networks (GNNs) for Mesh-based Simulations [5; 6]: Use GNN as a surrogate model for mesh-based solvers, with adaptive mesh refinement and high-dimensional message passing between the graph nodes.
   - Challenge: Adapting this framework to DFT. Transfer learning for generalization across multiple atomic configurations.

The physics applications for this line of research include accurate simulations for systems under extreme conditions such as planetary interiors and inertial confinement fusion reactors. Such ML aided solvers would enable on-the-fly modeling of the electronic response properties of samples in high energy experiments and would allow fast simulations that generalize well over input parameters of the experimental setup. The methods I develop can also potentially be used to create faster partial differential equation solvers applicable to other simulation-based fields.

I am also interested in studying the equivalence between Neural Networks and Gaussian Processes. During my internships [7] at the Lawrence Livermore National Laboratory, I worked on solving the inverse problem of inferring cosmological parameters from mass distribution in cosmological surveys using Neural Network Equivalent Gaussian Processes (NNGPs) [8].

I received my MS in Computational Science & Engineering and BS with double major in Physics and Computer Science from the Georgia Institute of Technology, Atlanta, USA. For my thesis, I worked on uncertainty quantification of neural network ensembles for DFT predictions [9].

Given my background, I was excited to read about the Les Houches Summer School this year (2022). Broadly speaking, exploring the synergies between physics and machine learning with the top interdisciplinary experts in the French Alps sounds like the perfect way to spend a month in the summer to me. I am looking forward to the following specific topics:

- PINNs: Optimization and regularization techniques to improve the convergence and stability of PINNs for increasingly sophisticated loss functions.

- GNNs: Message passing for high-dimensional high-fidelity surrogate models.

- Neural Tangent Kernels (NTKs): Utility of NNGPs/NTKs as surrogate models with uncertainty quantification for Density Functional Theory workflows.

- Interpretability and uncertainty quantification of deep learning models for natural science problems in general.

I believe that my research interests are well-aligned with the scope of the school, and learning from the top experts in the field in a summer school setting will help me in my goal of designing machine learning accelerated solvers for high-dimensional computational physics applications.

Thank you,
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