Statement of Purpose

Khalid Hossain
Postdoctoral Appointee, Leadership Computing Facility
Argonne National Laboratory

I have started as a postdoctoral appointee in the ALCF division at Argonne in the beginning of 2023. My primary responsibilities include developing and doing performance analysis of scientific applications running on large distributed computational platforms. During the course of my graduate studies I gained experience in doing HPC calculations in Summit at Oak Ridge. These calculations involved diagonalizing Hamiltonian matrices for superfluid systems and simulate dynamics of turbulent states. I prepared the initial states and wrote job scripts to complete the calculations. Beside that, I was introduced to performance analysis and scaling behavior of an application. Accurate analysis of performance and behavior of an application in a distributed environment requires deep understanding of the hardware and the communication between processors. Attending hands on sessions on MPI, OpenMP and scientific/numerical software design will be of crucial importance for my medium and long-term career goals. A large part of scientific computing is data analysis and visualization, specially for large simulations where tasks need to be done in the HPC environment. I have experience of performing such tasks but attending sessions at ATPESC and having a chance to speak with experts will be instrumental in the pursuit of my scientific interests. Overall, ATPESC will broaden the horizon of my computational knowledge by introducing new ideas, trends, techniques and applications which is crucial for my growth as a computational scientist.

Previous Experiences

As part of graduate studies I have simulated quantum turbulence – generation and dynamical evolution of turbulent states in superfluid systems. The goal was to develop experimentally relevant methods to reliably generate turbulent states and explore decay mechanisms for these quantum states. In ordinary fluids the decay of a turbulent state is attributed to the presence of viscosity which is absent in its known form for superfluid systems. We have validated different processes involving interactions between quantized vortices which gives rise to an effective viscosity facilitating the decay [1].

Simulating experimentally relevant volumes require leadership class computing facilities because of the size of the associated states. As an extension of the physics problem discussed above we have done work on Summit, hosted by Oak Ridge national laboratory. There we have ran successful simulation of a fermionic superfluid system with 72^3 lattice, where we diagonalized a $746,496^2$ Hamiltonian matrix to get the minimum energy turbulent state and then performed subsequent time evolution using Adam-Bashforth-Moulton (ABM) predictor corrector method. The diagonalization calculation was distributed over 512 nodes with 3072 processors for 8 self-consistent iterative loops. This is one of largest runs for such systems. We also attempted a 96^3 diagonalization, where the matrix size is $1,769,472^2$, requiring $3072 - 4000$ nodes with $18432 - 24000$ processors for 2 self-consistent loops. This was the first time we had a chance to explore the behavior of our code at such a large scale. During 96^3 diagonalization we saw a degradation in performance, and could not obtain a converged initial state for time evolution. For 72^3, we had almost ideal scaling behavior and expected performance. We are proceeding with 72^3 analysis, as it is sufficient to obtain physics results, 96^3 would be an improvement in statistics. One of the skills that I would like to learn by attending ATPESC is how to profile performance at such large scales, which are optimal performance and debugging tools and how to use them – leading to an understanding of the degradation of performance and failure of convergence for the 96^3-run, for example.

This work has been done as part of an ALCC project [2]. We have used a custom time-dependent density functional theory (TD-DFT) based on superfluid local density approximation (SLDA) functional.

The primary code is written using CUDA for GPU processing, MPI for parallelization and ELPA linear algebra libraries for diagonalization. This code has been released publicly as WSLDA toolkit [3, 4].

My primary responsibilities were to prepare seed initial states for the diagonalization, job submission and scheduling scripts via batch jobs (using `BSUB` and `jsrun` commands), ensure successful completion of simulations and perform data analysis by developing effective theories and models for turbulent dynamics in superfluids.

Research Plan

In my current position, my research plans can be divided in roughly three assignments. These involves performing Deep Learning (DL) research using computational resources in an optimal fashion. To that end, one of my short term research plan is to complete a performance analysis for different available frameworks (PyTorch, Tensorflow) used in different applications (convolutional networks, graph networks etc.) with varying degree of precision (fp32, tf32, bf16 etc.). Another major aspect of this analysis is to find area of improvements in cases of single-node, distributed and very large distributed network performance. The success of this project depends on a deeper understanding of distributed programming using MPI or OpenMP. The ATPESC workshop provides a solid foundation in that direction.

One of my long term projects focuses on DL applications in nuclear physics, more specifically calculating ground state and static properties of a nucleus using Variational Monte Carlo (VMC) techniques. The simplified idea of VMC is to begin a calculation sequence with an estimate of the ground state energy, and then minimize that to reach to a minimum energy state within acceptable accuracy. To make an initial estimate of the energy of the collection of nucleons we need to use an ansatz for the many-body wavefunction – this is a function of a few physical parameters which describes the distribution and density of particles. We will be using neural networks to make these ansatz and use them to facilitate the calculation of different physical properties. The current state of the art solves the problem for nuclei up to $A = 6$, where A is the total number of neutrons and protons in a nucleus [5, 6]. In these systems the typical number of trainable network parameters are on the order of $\sim 10^4$, and our goal is to extend the calculation to bigger nuclei, up to $A = 20$. For such large systems it is imperative that we take the advantage of distributed computing. We will be performing these calculations in leadership class facilities like Polaris and Aurora, hosted by Argonne national laboratory. I will be actively contributing in validating and developing code to get physics results along with the development of a benchmarking metric to compare performance across different hardware setups. Attending sessions on DL methods and training large models using distributed computing will be pivotal to the success of this project.

I will be actively working on another long-term project where the goal is to bring in interesting quantum simulations for the supercomputer Aurora. In the initial step this could be an extension of my work related to quantum turbulence. The work may involve direct porting of the WSLDA application to Aurora by converting it from CUDA to DPC++ (compatible with Intel GPUs) and exploring possible implementation with python frameworks like PyTorch, TensorFlow and Jax. Along the same line of developing quantum applications, I also plan to explore many-body entanglement using random matrix theory with potential application of DL methods. To improve on the performance of the WSLDA application, we may have to introduce different type of non-linear iterative solvers and numerical methods, ATPESC sessions on these topics will have significant impact of my progress in the right direction.

References

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