Blurb for the letter

February 23, 2023

Khalid has started as a postdoc at ALCF on January, 2023. He got his PhD in physics from Washington State University. In his graduate school years he worked on developing scientific software to simulate quantum dynamics of superfluid systems. These were density functional theory (DFT) implementations using Python. A significant part of his dissertation work was dedicated to reliably generate and study turbulent states in fermionic superfluid systems. Apart from being interesting in their own right as quantum simulators, superfluid dynamics have applications in nuclear astrophysics, specially in discussing pulsar glitches which are not fully understood yet.

Simulating fermionic quantum systems in experimentally relevant volumes is computationally challenging because of the size of the associated states. Therefore these become interesting test cases for leadership class facilities like ALCF, OLCF etc. Subsequently Khalid worked as a trainee graduate student in an ALCC project where he has performed large scale simulations in Summit at Oak Ridge.

Briefly, the computational task was to diagonalize a Hamiltonian matrix using self-consistent iterative methods to get the minimum energy state of the superfluid system within desired accuracy. Once the initial state has been acquired, the time evolution is performed to produce a turbulent state and study it's decay and other dynamic behaviors. It is imperative to have a good seed state for iterative solver to produce a promising initial state for the dynamics. Khalid was responsible for making these seed states, writing the job scripts and ensuring the successful completion of a simulation and optimal usage of their allocation time to make a campaign worth significant scientific value. He has actively contributed in developing effective models for these system to analyze the data from direct numerical solutions of the partial differential equations that describe the dynamics.

During the course of the ALCC project, Khalid was exposed to performance analysis and scaling behavior of a scientific application. Although he has not dived deep, this is where he wants to start his future endeavors of becoming a computational scientist. Various training tracks at ATPESC, ranging from MPI and OpenMP based distributed computing, advanced debugging and benchmarking to scientific software designing will give him a boost forward.

He has also worked as a summer intern at Lawrence-Livermore where he has worked with deep learning (DL) methods applied to nuclear fission problems. Through this work he has developed interest in DL methods, and he is currently working on a project to calculate different static properties of a nucleus using such methods. Attending sessions at ATPESC on DL methods and training large models in a distributed computing environment will significantly increase his chance of success.

Khalid wants to pursue a career as a computational scientist, where he would work with domain scientists to enable them in leveraging the resources available at leadership class facilities to tackle important problems. He has shown promise and it would be a great opportunity for him at the

early stage of his career to have exposure to new ideas and trends discussed at ATPESC while establishing connections with leading experts in the field.