Advanced Computing Training Program
Final Report

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The Texas Advanced Computing Center is currently one of the world's leading centers in High-performance computing, a status achieved throughout the years with a blend of knowledge, user-oriented philosophy and a seamless work environment. The multitude of teams composed of top-level and collaborative experts, span over different fields of responsibility, from hardware to software-oriented ones, covering areas from storage and algorithms to cloud-computing and visualization.

After the initial contact with my supervisor, Dr. Bill Barth, and a discussion on a possible training plan for the period, it was determined to fit me in within the High-Performance Computing team, where I would get the support needed from experts during the initial stages of the training program. In short, aiming towards my personal research interests in quantum optics and high-performance computing, but also making the most of the TACC's resources and expertise, was established a three-phase plan:

1. Training phase: The objectives of this phase were to establish a basic but solid knowledge of distributed computing programming frameworks, both in OpenMP and MPI, as well as an understanding of the computing systems available at TACC, in particular of Stampede 2 and Frontera. While the initial plan of attending the short courses offered by TACC backfired due to the lack of courses that were offered during the training period, a solution was quickly provided in the form of the online courses in the learn.tacc portal and existent online documentation. During this stage, I followed a series of interesting courses in OpenMP and MPI from basic to advanced level, as well as other courses about different optimization strategies. These courses, together with some real-time and personalized help and answers I got from many of TACC's researchers, helped me accomplishing the objectives set for this phase towards the end of the third week.

2. Development phase: This phase consisted of a hands-on project I have proposed to my supervisor before my arrival. In very few words, the project consisted of the development of a many-particle a high-performance simulation tool for quantum gases, a cutting-edge problem in quantum optics that allows to explore the uncharted complexity of the non-equilibrium regime. Starting from the development of small prototypes in Python and rapidly evolving to an implementation in C++, the code was developed in a serial framework and upgraded to work in a parallel environment with just one processor using OpenMP. After these successful steps, I focused my efforts on scaling the simulation tool to work on the massively parallel computing systems offered at TACC, first with a pure MPI approach and after that with a hybrid OpenMP-MPI approach, exploiting the shared memory in order to reduce the

memory footprint of a simulation. In this phase, I had the help of both Dr. Victor Eijhkout and Dr. João Barbosa, which helped me to structure the code, as well as in compiling strategies for the first runs and tests on Stampede2. This phase was completed towards the end of the fifth week.

3. Exploratory phase: The final phase was designed to be a flexible all-around period, exploiting the resources and competences of the center. In particular, I have focused on two distinct themes, performance and visualization. Regarding performance, the aim was to understand typical performance metrics used in the high-performance computing field and to perform some tests to my code. After discussions with some of TACC's experts, these tests brought interesting and unexpected results, which allowed to further optimize the simulation tool developed before and correct some bugs. On the other hand, for the visualization tasks, I once again followed some of the provided online courses that allowed me to become familiar with the concepts of the breakthrough areas of software-defined and in-situ visualization. On top of that, discussion with some of the staff of the visualization team introduced me to hierarchical data formats, a crucial strategy for simulation tools that exploit distributed memory and computing environments. Furthermore, towards the end of my stay I was able to use Stampede2 in server-mode for the post-processing of the results of some preliminary exploratory problems, that resulted into a couple of visualizations later analyzed at the Stallion, at the VisLab (examples: https://vimeo.com/368433430 and https://vimeo.com/368428129).

Parallel to these activities, I also had the opportunity to attend the TACCSTER conference, a series of short courses offered (Interactive Parallelization Tool, Pandas), and to participate in the regular staff meetings, which must be said, reflect the efficient and well-organized structure at TACC. Outside the research center, I must mention the quantity and quality of events happening at the University of Texas every week, which I had the opportunity to attend some advanced seminars at the Physics and Nanoscience departments.

Overall, the highly positive impact of the ACTP can be analyzed in two different topics. First, on the personal side, the program provided me an opportunity to fill some gaps of my skills-set, which without a doubt opens me new doors and trails new paths that can materialize into a great kick-start for a long-term scientific career that I pursue. I am also sure that this great opportunity to establish in-situ a network in one of the most advanced research centers will reverberate positively in short and medium-term, with collaborations and hopefully high-quality research projects. On the other hand, I believe that the knowledge I am bringing will be an important asset to consolidate a strategic vision of the research group I belong to, and that will help to establish the Centre for Applied Photonics group of INESC TEC at the upfront of groundbreaking fundamental research in photonics at the international level. Besides, once returned, I will try to generate value by conducting a series of courses to pass some of the most recent knowledge in supercomputing trends to the future generations of students and researchers.

To finalize, my overall impression: working at TACC was a great experience, not only due to its cutting-edge technologies but mostly due to their collaborative and open-minded teams, always available to help users from a wide scientific community to access the potential of high-performance computing. On top of that, Austin is a friendly city, with a vivid culture, great places and good weather, which ultimately provides a great balance between a state-of-the-art work environment and high-quality living style.