Undergraduate Summer Research in High Performance Computing with Engineering Applications: An Experience Report

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Abstract

High Performance Computing (HPC) stands at the forefront of engineering innovation. With affordable and advanced HPC resources more readily accessible than ever before, computational simulation of complex physical phenomena becomes an increasingly attractive strategy to predict the physical behavior of diverse engineered systems. Furthermore, novel applications of HPC in engineering are highly interdisciplinary, requiring advanced skills in mathematical modeling, algorithm development as well as programming skills for parallel, distributed and concurrent architectures and environments. Reasons such as this have created a shortage of qualified workforce to conduct the much-needed research and development in these areas. This paper describes our experience with mentoring a cohort of ten high achieving undergraduate students in Summer 2019 to conduct engineering HPC research for ten weeks in Clarkson University. Our mentoring activity was informed and motivated by an initial informal study with the goal to learn the roles and status of HPC in engineering research and what can be improved to make more effective use of it. Through a combination of email surveys, in-person interviews, and an analysis of faculty research profiles in Clarkson University, we learn several characteristics of their research. First, a large proportion of the engineering faculty conducts research that is highly mathematical and computational and driven by disciplinary sciences, where simulation and HPC are widely needed as solutions. Second, due to the lack of resources to provide the necessary training in software development to their students, the interviewed engineering groups are limited in their ability to fully leverage HPC capability in their research. Therefore, novel pathways for training and educating engineering researchers in HPC software development must be explored in order to further advance the engineering research capability in HPC. With a three-year support from NSF, our summer research mentoring activities were able to accommodate per year ten high-achieving undergraduate students recruited from across the USA and their faculty mentors on the theme of HPC applications in engineering research. In this experience report, we describe our first offering of the site in summer 2019, including the processes of students recruitment and selection, training and engagement, research mentoring, and professional development for the students. Best practices and lessons learned are identified and summarized based on our own observations and the evaluation conducted by an independent evaluator. In particular, improvements are being planned so as to deliver a more holistic and rigorous research experience for future cohorts.

I. Introduction

High Performance Computing (HPC) stands at the forefront of engineering innovation [1, 2]. With affordable and advanced HPC resources more readily accessible than ever before, computational simulation of complex physical phenomena is an increasingly attractive strategy to predict the physical behavior of diverse engineered systems [2], such as systems in nuclear safety [3], outcome of cancer treatment [4], or multidimensional flight stresses on aircraft. To maintain the U.S.'s leadership position in HPC production and application [2], and to meet the needs of the rapidly growing HPC market [5], American institutions of higher education must produce a sufficient supply of highly-trained HPC professionals. Sadly, at current rates of enrollment and graduation, U.S. institutions will fall short of producing the needed HPC professionals [6]. Worse yet, groups largely untapped by this field, women and minorities, make up a significant portion of the nation's growing talent pool [7], but are extremely underrepresented in HPC related disciplines.

A Research Experiences for Undergraduates (REU) Site is an important mechanism to combat the shortage of HPC professionals. The REU program by the U.S. National Science Foundation (NSF) supports active research participation by undergraduate students in any of the areas of research funded by the NSF. REU projects involve students in meaningful ways in ongoing research programs or in research projects specifically designed for the REU program. As one mechanism of the REU program, REU Sites are based on independent proposals to initiate and conduct projects that engage a number of students in research. REU Sites may be based in a single discipline or academic department or may offer interdisciplinary or multi-department research opportunities with a coherent intellectual theme. An REU site provides an opportunity for talented undergraduate students to spend 8-10 weeks to engage in full time research under the supervision of experienced faculty and graduate mentors. In this paper, we describe our experience with running the first year of a three-year HPC REU site in the summer of 2019 on the campus of Clarkson University. The goal of our REU site was to *encourage talented undergraduate students to pursue graduate study and HPC careers by engaging them in exciting and meaningful research experiences and by cultivating their talents during their summer experiences and beyond.* To address this project goal, our REU site pursued three objectives:

1) Engage a total of 10 students annually from traditionally underrepresented groups or from colleges and universities with limited research opportunities, immersing these students in ongoing research projects in HPC-related engineering fields.
2) Cultivate talented students to effectively plan, conduct, and communicate scientific research through meaningful and engaging research projects, close and effective mentoring, weekly group meetings, mentor training, and public presentations.
3) Improve educational pathways to advanced HPC-related careers through student involvement in field trips, expert speaker series, and additional professional development activities.

The rest of this paper is structured as follows. Section II presents related work. Before launching our HPC REU site, we conducted a survey to understand how HPC is currently utilized in engineering research at Clarkson University and what can be done to improve HPC education and training. Section III presents a summary of the main characteristics that we learned about the research of our faculty members with respect to HPC. Section IV introduces our new NSF REU site regarding HPC applications in engineering research at Clarkson University and the operation of its first summer session in 2019. Section V summarizes the good practices and lessons learned through analyzing the program evaluation results. Lastly, Section VI concludes the paper.

II. Related Work

U.S. government has invested significantly in the HPC facilities of universities. For example, in August 2018, NSF awarded $60 million for the next generation supercomputer (to UT Austin) [8]. However, an HPC research ecosystem requires not only the hardware but also training and education in software programming and optimization. Otherwise, the advanced HPC hardware cannot be fully utilized. In fact, United States Council on Competitiveness states that while most U.S. government labs have training programs and programs for outreach, they are not as well done nor as well staffed as they could be [9]. The problem is in programming skills needed for HPC. Users of HPC facilities must port their applications to take advantage of these large-scale systems.

Hannay et al. investigated how scientists develop and use software in their research based on an analysis of results from a large on-line survey [10]. They found that, while many respondents do computational modeling, only a small proportion of them use HPC. Furthermore, they found that most respondents are not formally trained for HPC software engineering and that many software engineering best practices may not be necessary for small-scale HPC projects. Heroux and Willenbring summarized 10 good software engineering practices to improve computational science and engineering software [11].

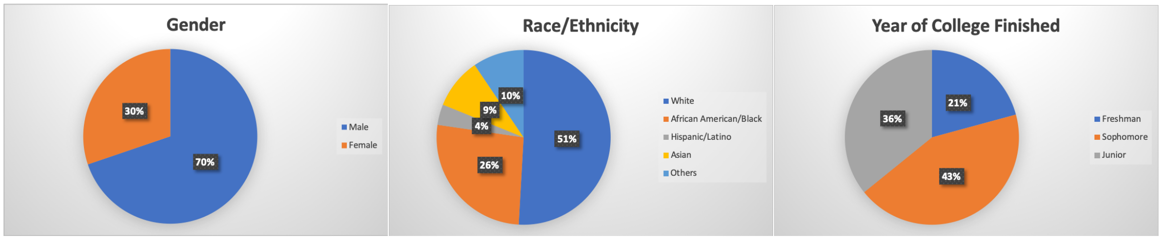
III. Survey of HPC Applications in Engineering Research at Clarkson University

Our survey methodology involves emails, in-person interviews of selected faculty members, and a manual analysis of all engineering faculty members' public research profiles at Clarkson University. In August 2018, we emailed 16 engineering faculty members asking them to describe their computational research projects. Based on their response, we concluded that engineering research at Clarkson University relied heavily on computational approaches, simulation, and mathematical modeling. Subsequently, to further expand our understanding of the use of computational modeling and HPC in research and to identify opportunities for improvement in education and training, we conducted more in-depth interviews with four of the faculty members initially surveyed. Table I summarizes the four interviewees' HPC research based on input from the interviews. Lastly, to develop an overview of the use of computation and HPC in engineering research at Clarkson University, we analyzed the research profiles of all 79 tenure-track or tenured engineering faculty members. Specifically, we checked the research interests of each faculty member as listed on their personal website. Furthermore, we read the abstracts of their research awards and recent publications. To further understand their research focus, we also consulted with their google scholar pages. We concluded that only five out of the 79 faculty members make full use of HPC in their research, but as many as 35 of them rely on computational modeling approaches in their research and thus could benefit significantly from leveraging HPC capability.

TABLE I: Example Applications of HPC in Engineering Research at Clarkson University

Faculty	Applications	Model	Computing Systems	Prog. Lang.	Grad. Student Background
Prof. C	Electron Transport Wave Propagation Thermal Behavior	PDEs	Multicore CPU PC	C/C++ Fortran Matlab	All Engineering and Math Major without Prog. Training
Prof. D	Magnetic Resonance Imaging Electromechanical Modeling	PDEs ODEs	Multicore CPU PC	C Matlab	Chemical Engineering with Limited Prog. Training
Prof. L	Multiphysic Sim. Framework Target Alpha Therapy	PDEs MC	Multicore CPU PC Computing Clusters	C/C++	Computer, Software Eng. Computer Science
Prof. W	Uncertainty Quantification Bld. Response to Wind/Storm	PDEs	Multicore CPU PC GPGPUs	C/C++ Matlab	Civil, Mechanical Eng. with Short HPC Training

In the following, we further summarize in three points the feedback from the interviewed faculty members about their research and use of HPC:



(a) Gender distribution (b) Race/ethnicity (c) Class standing

Fig. 1: Demographics of the 53 applicants received by the Clarkson University HPC REU Site in 2019.

Point 1: Both the faculty researchers and their graduate students are short on professional training regarding the use and development of HPC techniques. Therefore, it is often difficult for them to develop full-fledged HPC applications by adopting and customizing state-of-the-art open source HPC tools (e.g., OpenFOAM [12], Geant4 [13]) or by developing their own in-house simulators to address their HPC needs. This is because the engineering researchers and students are unfamiliar with the specific parallel and distributed programming models that the HPC tools are based on. In addition, due to the lack of specific programming skills, the researchers usually prefer to using existing commercial tools, such as Matlab [14] and ANSYS [15]. These tools have the basic capability of distributing scientific computing work to multiple computing units. However, their license cost can be too high for our faculty to afford when large-scale HPC computing is requested.

Point 2: Due to the reasons above, faculty researchers are forced to create small scale simulations and models that can only be run on a single commodity computer. Most researchers in the Wallace H. Coulter School of Engineering at Clarkson University only work on small-scale or simplified scientific computing scenarios due to the computational complexity of large-scale simulations and extremely high cost of commercial tools. To further their research into large-scale simulation required in real-world scenarios, HPC techniques can be applied to optimize their research computing code in the future.

Point 3: The engineering faculty tends to recruit graduate students from their respective engineering disciplines. The advantage of this practice is that these students are well prepared for working on the engineering problems. The downside is that they are rarely formally educated enough in skills required for developing HPC software. Novel educational pathways must be explored to better prepare these students in computational approaches and HPC software engineering that are increasingly becoming critical for engineering research.

IV. NSF REU Site on HPC at Clarkson University

Based on the findings listed in Section III, it has become evident to us that there are strong needs and willingness among our faculty members to mentor undergraduate students in conducting HPC-based engineering research. Motivated by these observations, we submitted an REU site proposal on HPC applications to NSF, which was subsequently awarded. In what follows, we summarize our experience with operating the REU site in the first summer (May 25, 2019 - August 2, 2019) on the Clarkson University main campus in Potsdam, NY.

Fig. 2: Participants of the NSF HPC REU site won a total of five awards (three best oral presentation awards and two best poster presentation awards) on August 2, 2019 in Clarkson University's 2019 bi-annual research conference RAPS (Research and Project Showcases).

Despite our tight schedule and late opening relative to other existing REU sites, with persistent advertisement efforts through multiple channels, our HPC REU site has managed to attract 53 applications from undergraduate students across the United States. Figure 1 depicts the distributions of the gender, race/ethnicity, and class standing of the applicants. These candidates were of sophomore or junior standing with a GPA of at least 3.0, coming from multiple academic majors, including engineering physics, mechanical engineering, chemical engineering, computer science, software engineering, applied mathematics, and computer engineering. As depicted in Figure 1, our REU site has raised the interest of students from diverse background, reassuring us that our original motivation inspired by our analysis of the current state of HPC education is on the right track.

After multiple rounds of careful application reviews by both site directors and the faculty mentors, ten students were selected and participated in this site in summer 2019. These students worked on ten HPC relevant projects prepared for this REU site. The conducted research projects, along with the mentors, are listed in Table II.

At the end of the 2019 summer program, all ten of our REU Site participants attended Clarkson University's bi-annual undergraduate research conference RAPS (Summer Research and Project Showcase) [16], each giving both an oral presentation and a poster presentation. Our participants won five awards, three on best oral presentations and two on best posters, a clear demonstration of the high-achieving quality of this cohort. Figure 2 shows a picture of the group taken at the award ceremony.

The ten students were from ten different universities majoring in multiple engineering disciplines and applied mathematics, and are distributed geographically across six US states (Mississippi, Kentucky, Ohio, Pennsylvania, New York, Connecticut). Consistent with NSF's expectation to promote diversity in the HPC talent pool, our selection gave priority to students of underrepresented groups and females as well as those who do not otherwise have access to research opportunities. As a result, 20% of the selected participants were underrepresented minorities, 20% female, and 60% from universities with limited research opportunities in HPC.

TABLE II: Research Projects for Clarkson University's HPC REU Site in Summer 2019

Mentor	**Project Title**
Dr. A, Chemical and Biomolecular Engineering	Uncertainty quantification and propagation for improving reliability of cardiac modeling and simulation
Dr. B, Mechanical and Aeronautical Engineering	3D CFD code for high-order accurate direct numerical simulations of single and multi-phase flow
Dr. C, Electrical and Computer Engineering	Multi-dimensional scaling (MDS) based SLAM solutions (Simultaneous Localization and Room Mapping)
Dr. D, Electrical and Computer Engineering	A reduced-order thermal model for thermal aware architecture design exploration of semiconductor chips
Dr. E, Electrical and Computer Engineering	Network dynamics with distributed computing
Dr. F, Electrical and Computer Engineering	Utilizing GPUs to speed up causation entropy modeling
Dr. G, Electrical and Computer Engineering	Benchmarking concurrent algorithms across parallel computing platforms
Dr. H, Electrical and Computer Engineering	Exploring an open source based benchmark suite for multi-physics engineering computing
Dr. I, Applied Mathematics & Electrical and Computer Engineering	Analysis of spatiotemporal dynamical systems from multi-attribute remote sensing
Dr. J, Mathematics	Forensic footwear print registration

In addition to the research projects, we also organized participant activities to support students' research and life in our site and to encourage their future applications to graduate programs. The main activities of our site in 2019 are listed as follows:

1. Mentoring workshop (Friday May 24, 2019): A two-hour mentoring workshop was led by the site directors. It had 12 faculty and graduate student mentor participants. Best practices in mentoring summer REU students were discussed.

2. An orientation session was held on Monday May 27, where the site directors, the Engineering Dean, Dr. William Jemison, and the ECE Chairman, Dr. Paul McGrath, welcomed our REU cohort with brief inspirational speeches.

3. Team building activities were provided to welcome the students and to familiarize them with the REU faculty team and with each other through a retreat and a high rope course at Camp Oswegatchie (May 30-31, 2019).

4. An HPC crash course was provided to our participants to cover the major HPC programming paradigms with hands-on lab exercises carefully designed to help reinforce concepts and consolidate learning. Besides our own lectures, students also participated in the

Extreme Science and Engineering Discovery Environment (XSEDE) summer online workshop provided by Pittsburgh Supercomputer Center (the 1st week of June, 2019).

5. Led by the site directors, weekly research group meetings were conducted on Fridays for the entire cohort, which provided an authentic environment to experience the research process in a structured context, to hone skills in both poster and oral presentation, and to stimulate peer learning and exposure to the broader set of projects.

6. Two technical field trips were organized for the REU cohort, including visiting the IBM HPC facility on the Poughkeepsie campus (June 27-28, 2019) and the Canadian Nuclear Laboratories (June 13, 2019).

7. A rich set of professional development activities were offered to our participants, including seminars from two invited speakers (Dr. Mike Welland of Canadian Nuclear Laboratories and Dr. Shuangshuang Jin of Clemson University, both experts in HPC applications), and five professional development seminars by Dr. Jon Goss, Head of Clarkson University's Honors Program ("Graduate school application process", "Secrets of a great personal statement", "Ph.D. dissertation research", "Managing your faculty mentor", and "Poster development and public speaking").

8. Program Assessment and Evaluation. The Clarkson University 2019 High Performance Computing (HPC) REU Site was evaluated with data collected through three surveys and two focus groups. The purpose of the surveys and focus groups was to gauge the attitudes, perceptions, and reactions of the student and faculty mentor participants. More on the results of the program evaluation will be presented in Section V of this paper.

V. Program Evaluation Results for Summer 2019

The Clarkson University 2019 High Performance Computing (HPC) REU program was evaluated with data collected through three surveys and two focus groups. The purpose of the surveys and focus groups was to gauge the attitudes, perceptions, and reactions of the student and faculty mentor participants. The analysis was undertaken to determine if the program's goals were met and to identify areas in need of improvement. An independent program evaluator, Dr. Patrick Turbett, Director of the Potsdam Institute for Applied Research [17] and Professor Emeritus of Sociology at the University of SUNY Potsdam, conducted and analyzed the results of the surveys and, with a PIAR staff member, conducted the focus groups.

Student participants completed a pre-program and a post-program survey and took part in two focus groups, one midway through the program and another at the conclusion of the REU program. Ten students participated in the program with ten faculty mentors. Ten students completed the pre-survey. Ten students completed the post-survey. Eight participated in the mid-way focus group (two students were absent due to personal reasons), and ten participated in the final focus group. Eight faculty mentor surveys were completed.

The student surveys were administered on-line at the beginning and end of the REU program. The "pre-program" survey focused on the students' prior experience with research projects and working with a mentor, their expectations for the REU program, their current perceptions of high performance computing, as well as their view of the importance of graduate study as a path to a career in basic or applied research and their intention to attend graduate school. The "post-program" survey solicited feedback on program activities and on their experience with their faculty mentor to determine the quality of the program. It also repeated key questions from the pre-program survey to determine any change in reported experience level, perception of HPC, the role of research and graduate schools, and post-graduate plans.

The focus groups served as another means of soliciting student feedback. The group discussed the success of the program, recommendations for improvement and ways the program supported future education endeavors.

The mentor surveys were administered as an online survey at the end of the program. The survey focused on the quality of the students, the quality of the research project, the team's success in completing the project, the mentor's satisfaction with the program and the administration of the REU program, and their understanding of the mentor role.

Through analyzing the anonymized, aggregated feedback data provided by the independent evaluator, several good practices and lessons learned have been identified for the future improvement of this REU site.

A. Good Practice–what we've been successful in doing

- HPC Crash Course: The education purpose of our one-week HPC crash course has been achieved, since in the post-survey our participants indicate that it is more than *significantly helpful*. In addition, we observe a clear improvement of the HPC knowledge in our participants through comparing their quiz scores in both pre- and post-survey, which are based on the exactly same set of 10 multiple choice questions on HPC topics. The average percentage of correct answers improves from 42% in the pre-survey, to 63% in the post-survey.
- Weekly Group Research Meetings: These required meetings during the lunch hours on every Friday are designed for students and the site directors to work collectively on defining a research proposal, reporting research progress, and preparing for presentation of research outcomes. Overall, REU participants are positive about the meetings, ranking many aspects of it as being *significantly helpful*. They rank the research proposal portion of the group meetings as *significantly helpful* in helping them with *understanding an important aspect of conducting research*, *effective communication of research results*, *holding my interest*, and *working with other people*. They rank the research progress tracking portion as *significantly helpful* in *understanding an important aspect of the research progress* and *effective communication of research results*, but less so in *holding my interest*. Lastly, they recognize the research communication component of the group meetings as *significantly helpful* in *understanding an important aspect of the research progress* and *effective communication of research results*.
- HPC Invited Speakers: Two invited speakers present HPC research in power engineering and nuclear engineering. Our participants indicate that the seminars from our two invited speakers are *significant helpful* for them to understand *an important aspect of conducting research* as well as *holding their interest of HPC relevant research*.
- Professional Development Workshops: Five one-hour workshops have been offered during the program. Overall students are positive about these workshops. For example, our participants believed that the workshop of PhD pathway panel and crafting personal statement are almost *tremendously helpful* for their decisions related to graduate school

and future. In addition, the workshop of polishing presentation is also ranked above *significantly helpful* to build their capacity of effective communication of research results.
- Field Trips: Our program offered three field trips in summer 2019. Our participants report that the first trip (high ropes training course) is very fun and has been effective in helping build rapport among themselves and with the site directors. The second trip (Canadian Nuclear Laboratories (CNL)) has achieved multiple goals by being *significantly helpful*, including aspects of general HPC education, teamwork, importance of HPC research, communication skills, and future career decision. The third trip to the IBM's mainframe site in Poughkeepsie, New York has also achieved similar effects in these aspects, but is reported to be especially effective in improving the students' understanding of the importance of teamwork.

B. Lessons Learned–what we'd strive to improve next summer

- Research Projects: According to the post-survey results, perhaps not surprisingly, our participants rank the *experience in conducting the research project itself* as the most important aspect in their overall summer experience, followed by *going to field trips* and *interacting with fellow students and mentors*. While they acknowledge that they've *learned a lot from participating in the research project*, they believe that future projects have opportunities to contribute more to an *increased understanding of HPC and engineering*. All projects are computational in nature, and some of our students are not comfortable with the amounts of mathematical, engineering or programming background required. Challenges like this take away time for practicing HPC skills. Above all, since the duration of this REU site is only a short 10 weeks, so mentors and site directors must be mindful of what can be reasonably accomplished during the 10 weeks and set the right expectation from onset for the REU students. The students' perception of success of the REU research projects listed above is very sensitive to the progress tracking and their well definition. The site directors is planning to work more closely with mentors in better scoping the research projects before students arrive. They also plan to screen the applicants more carefully to match students with the right projects as well as providing stronger support and training to the students through the crash course.
- Mentoring: Overall, our participants have given positive evaluation in the post-survey results of their interactions with mentors. In particular, in a Likert scale from 1 to 7, they *strongly agree* that their mentors should continue with project mentoring in the future. However, due to faculty members' busy schedule, the site directors have also observed that a small number of mentors are not prepared well to coach students in the summer. Recognizing that mentor commitment is very important to site success, in the future, the directors plan to be more explicit with a prospective mentor about the required time and effort commitment. In addition to continuing to hold the mentoring workshop in the week before the REU site is open, more conversation and interviews between the site directors and the mentors when the site is in session during summer, could also be effective, as it can be helpful to remind and encourage our mentors to fulfill their commitment and give timely feedback and guidance to our REU participants.
- Crash Course: An important objective of this REU site is to bridge the HPC education gap between engineering majors and computer and software majors. Thus, inevitably the participants of this REU site has diverse backgrounds. Consequently, timely and on-demand training of supporting techniques is necessary to increase the likelihood of the

success of the REU site. For example, many engineering projects require the knowledge of numerical algorithms like solving Partial Differential Equation (PDE) equations. Therefore the introduction to a library such as Portable, Extensible Toolkit for Scientific Computation (PETSc) can be very beneficial to the students. Adding such training to our crash course, and above all, making the crash course dynamic and more adaptive to students' research needs, can be useful to our future cohorts.

VI. CONCLUSIONS

We report on a preliminary analysis of the use of computational modeling and HPC in engineering research based on the research activities at the Wallace H. Coulter School of Engineering at Clarkson University. While we see great potential of computational modeling and HPC in enabling cutting edge engineering research, we also conclude that novel pathways for better preparing engineering researchers in their software engineering capability must be explored to further advance engineering research capability. These findings have been put into use in our newly awarded REU site supported by the U.S. NSF, with a theme on HPC applications in engineering research. Best practices and lessons learned have been identified and summarized based on the experience and the evaluation results of the first running of the site in the summer of 2019. Although this paper contributes only a single case study, we hope that it can be used to improve future REU sites and undergraduate research in general.

Overall, while we have seen clear evidence that our REU site has succeeded in providing a fun and engaging environment for conducting enriching REU research in the summer, we have also identified opportunities to improve our program such that more REU students can successfully complete the projects that they've defined for themselves in the onset of their summer program (higher project completion rate). To deliver a more holistic research experience for future REU cohorts, the site directors are planning to (1) work closely with prospective mentors to provide better defined projects and ensure that they are feasible for an undergraduate student to complete in a 10-week time frame, (2) identify stronger students with background that are better prepared for conducting the proposed research projects, and (3) conduct better planned, more agile HPC training crash course that is more adaptive to the needs of the summer research projects, which will require more proactive planning on the part of the site directors.

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