The Blue Waters Petascale Institute: Longitudinal Impact and Assessment-Driven Development of an Intensive, Hands-on Curriculum for Teaching Applications in HPC

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ABSTRACT

The Blue Waters Petascale Institute was a two-week intensive training program that ran annually from 2014–2018. The institute implemented a hands-on, inquiry-based approach comprised of exploratory activities, engaging discussions, and informative lectures. These allowed students to learn parallel programming, high-performance computing, and computational science concepts with relevant examples from a wide range of real-world, domain-specific applications and scenarios. The goal was to provide undergraduate and beginning graduate students with the background and skills necessary to be successful not only during the institute but also in year-long research projects and into their future academic and professional careers. This paper examines the longitudinal impact of the institute on its students and recounts how the institute curriculum evolved over time based on formative and summative assessments. Results show that, overall, students considered the institute a positive experience and felt they gained the confidence and knowledge necessary to be successful in their internships and in their future careers. The institute has made a lasting impact in providing students with the ability to produce top-notch research outcomes of publishable quality, and students have taken what they learned into graduate programs, industry positions, and other career directions.

CCS CONCEPTS

• **Social and professional topics** → **Model curricula**; *Computing education*; *Computational thinking*;

KEYWORDS

Blue Waters Petascale Institute, Blue Waters Student Internship Program, Extreme Science and Engineering Discovery Environment (XSEDE), XSEDE EMPOWER Program, HPC Undergraduate Education, Applications in HPC, Curriculum Development, Evaluation, Impact, Computational Science Education

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1 INTRODUCTION

The Blue Waters Petascale Institute ran for five years (2014–2018). On average, 28 students participated each year, ranging from first-year undergraduate to beginning graduate students from various Science, Technology, Engineering, and Mathematics (STEM) disciplines. Nearly all students had little to no background in high performance computing (HPC) and parallel programming. Most of the students were undergraduate interns participating in the Blue Waters Student Internship Program (BWSIP). For these students, the institute provided the parallel programming and HPC tools, confidence, and knowledge necessary to be successful in a year-long research project at the conclusion of the two weeks. Besides the BWSIP, some students also came from the student programs of the Extreme Science and Engineering Discovery Environment (XSEDE) [17].

As part of the institute, students were given access to Blue Waters, one of the world's most powerful supercomputers [4]. Lessons and labs were designed to make use of hands-on access to its many-node, CPU and GPU hybrid architecture. By virtue of working with Blue Waters, students also received expert assistance from the applications support staff at the National Center for Supercomputing Applications (NCSA). Both Blue Waters and NCSA are housed on the University of Illinois at Urbana-Champaign (UIUC) campus,

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Figure 1: Students’ departments by year. “N” is the number of students in each year. “Engin. Discipline” represents a category of various Engineering departments such as Aerospace, Civil, Environmental, Mechanical, Materials Science, and Petroleum Engineering. Note that Chemical Engineering is grouped under “Chemistry” rather than “Engin. Discipline.” Student departments categorized under “Other” included Philosophy, Psychology, Computational Science, and STEM. Students for whom we did not have department data are listed under “Unknown”. Students from joint departments were included fractionally in each category (e.g. a student from a department of Physics, Mathematics, and Computer Science was counted 1/3 in each category).

and hosting the institute at this venue allowed the students to see the machine in person and interact directly with the NCSA staff. This provided a supportive learning environment and a welcoming introduction for students new to HPC. This paper focuses on the success of students participating in the institute, how it made an impact on their academic and professional careers, and how the curriculum evolved from year to year based on formative and summative assessments.

2 STRUCTURE OF INSTITUTE

Each iteration of the institute was comprised of about 80 hours of instruction time spread over two weeks. The 80 hours included about 40 hours of core lectures and hands-on exercises for inquiry-based exploration as well as around 20 hours of evening labs for reinforcing the concepts students learned throughout each day. Five to ten hours were allotted for invited speakers who shared advice and insights from careers in HPC, such as tips for applying to graduate school, project management, and representation of women in HPC. Finally, 10–15 hours were designated for the students to start applying what they had learned to their individual research projects, with instructors and Blue Waters applications support staff providing one-on-one support. More details of the structure and content of the initial 2014 institute are given in [13], and the agenda and materials for each year’s institute are posted online at [1].

A typical day of the institute began with an introductory computational thinking activity designed to “launch” the main topics

of the day, followed by about 8 hours of core lectures, hands-on exercises, and guest speakers (also including an hour lunch break and two 10–15 minute breaks), concluding with a two-hour evening lab after dinner to tie together the main topics of the day.

While some students gave feedback over the years that this was an exhausting schedule, and some said they would have preferred either covering the same amount of material over three weeks or otherwise cutting back on the amount of material covered in two weeks, there were a number of benefits to the two-week schedule. Most importantly, including two weeks of material instead of just one allowed us to cover a wider depth and breadth of topics: not just parallel programming but also complementary topics like optimization, automation, visualization, research project management, and career planning. In addition, an intensive schedule encouraged everyone to treat the two weeks as a focused, “boot camp”-style learning experience (in contrast to an extended seminar-style event where students passively listen to lectures during the day and disengage in the evening). Finally, keeping the students together for two intense weeks fostered a community that persisted past the duration of the institute and led to a sense of belonging in the field of HPC.

2.1 Location

Each year’s institute was held at NCSA on the UIUC campus in late May or early June. While students came from all over the U.S., and most would ultimately complete year-long internships at their home institutions, bringing students together for the two-week

Figure 2: Average Blue Waters Interns' self-scored experience with HPC (N = 98) and parallel programming (N = 97) prior to the institute. Interns were asked to gauge their experience with the topics on a scale of 1 (Inexperienced), 2 (Novice), 3 (Competent), 4 (Proficient), and 5 (Expert). While individual values ranged from 1-5, no averages exceeded 2 (Novice).

institute provided them with the ability to meet other interns, tour the National Petascale Computing Facility (NPCF, home of Blue Waters), and network with experts in HPC and related fields from NCSA and UIUC.

2.2 Participants

The institute was designed primarily for interns participating in the BWSIP; however, XSEDE also found it valuable to have students from their programs participate. Each year, students from the following XSEDE programs participated:

2014 XSEDE Summer Research Experience (SRE): 2 undergraduate and 2 graduate students

2015–2016 XSEDE Scholars Program (XSP): 10 graduate students each year

2017–2018 XSEDE Expert Mentoring Producing Opportunities for Work, Education, and Research (EMPOWER) Program: 5–6 undergraduate students each year

Beginning in 2015, select students were also invited to participate in the institute each year who had submitted high-quality applications to the BWSIP but were otherwise not eligible to be funded as BW interns, such as beginning graduate students or additional undergraduate students for whom there was not adequate funding to support an entire year's worth of research stipends. This included:

2015 2 undergraduate and 3 graduate students

2016–2017 2 undergraduate and 2 graduate students each year

2018 2 graduate students

The BWSIP selection process for applicants aimed, among other things, to choose interns who would benefit the most from the

institute.¹ The goal was to provide this experience to students who had a strong foundation in their various domain disciplines (see Figure 1). In most cases these students had some serial programming experience but might otherwise have not had an opportunity to learn how to apply HPC and parallel programming to their research. While many students came from computer science departments, over time this percentage declined from 51% in 2014 to 19% in 2018. Conversely, over the years, other departments became more represented, including Chemistry and Engineering, which had no representation in 2014. As shown in Figure 2, the BWSIP intern pool from each year self-identified as having on average less than “Novice” experience in HPC and parallel programming. This meant that, even if students attending the institute had general programming experience, there was still a gap in their knowledge of HPC and parallel programming on average.

Applications to both the BWSIP and XSEDE programs were encouraged from women, minorities, and people from other groups underrepresented in STEM and HPC, but underrepresented status did not factor into the selection process for these programs (and indeed names, genders, and ethnicities were redacted from applications wherever possible during the review process in an attempt to avoid bias). Students had the option to identify their gender and ethnicity on their applications only for data collection purposes; these data are shown in Figures 3 and 4, respectively. On average we had 29% female students, which is above the 5–17% of users, researchers, and conference attendees in the HPC field [18]. On average we had 20% of students identifying with ethnicities considered underrepresented in STEM, which is close to the 22% of science and engineering bachelors degrees earners who are underrepresented minorities, and it is well above the 9% of science and engineering doctorate degree earners who are underrepresented minorities [11]. A diverse group of students contributed to a positive learning environment. One student commented on an exit survey, “I felt really loved and taken care of by everyone and overall I am constantly amazed by how diverse the Institute is.”

¹For more details on the selection process, see [13]

Figure 3: Student genders each year at the institute. The total number of students each year are given in Figures 1 and 4.

Figure 4: Student ethnicity categories by year as indicated by students on applications to the BWSIP or XSEDE programs. “N” is the number of students in each year.

2.3 Instructors and Guest Speakers

When the first institute was taught in 2014, the core instructors were all staff from the Shodor Education Foundation, Inc., in Durham, North Carolina (including authors Aaron Weeden and Mobeen Ludin), with some topics taught by guest lecturers from NCSA and UIUC. With the next institute in 2015, Shodor added a student to the instructional team who had just completed her year-long research project as a Blue Waters Intern (author Colleen Heinemann). In subsequent years, additional student instructors were added to the team from the previous pools of Blue Waters Interns (including author Cameron Foss) and XSEDE Scholars, as well as additional Shodor staff and frequent Shodor collaborators (including authors Jennifer Houchins and Skylar Thompson).

The pipeline of students-turned-instructors not only demonstrated an effective curriculum but also gave current students first-hand insight into the program’s expectations from “near-peer mentors” who had recently completed the program themselves. The student instructors increased the diversity in the academic backgrounds of the instructional team; whereas the Shodor staff came primarily from Computer Science, the student instructors came from backgrounds of Astrophysics, Computational Chemistry, Electrical Engineering, Mathematics, and High-Performance Visualization. This wide range of knowledge from the instructors led to richer and more varied examples for exercises and lectures and enabled more of the students to have their domain-specific questions answered by the instructors. By recruiting a group of experienced student instructors from diverse disciplines, the instructional team reflected the diversity of the students’ disciplines. With the addition of student instructors, the sustained student-instructor ratio (not counting guest speakers who were only present for one session as opposed to full weeks of the institute) decreased from 7:1 in 2015 to 5:1 in 2016 to 4:1 in 2017 to 3:1 in 2018 (across all five years, the

average was 5:1).² These decreasing ratios made it easier for the students in later years to receive more personalized attention and get help faster than for students in previous years.

Even with an expanded number of student instructors, guest speakers from NCSA and UIUC remained an important part of the institute. After 2014, rather than having the guest speakers lecture about core topics like parallelization or GPGPUs, the speakers were instead invited to provide career insights and advice. For example, Dr. Daniel Wong from the Graduate School at UIUC was invited in 2017 and 2018 to talk about graduate education to the students. In both years, his session was rated among the highest of any session at the institute; in neither year did any student rate the value of the session less than “somewhat valuable”, with nearly all students rating the session as “extremely valuable” [7]. Lastly, staff from the Blue Waters Science and Engineering Application Support (SEAS) team were always on site in-person to address any questions or issues discovered by the instructional team, such as technical problems with the Blue Waters machine or questions about best practices in parallel programming and optimization.

3 EVALUATION AND IMPACT

3.1 Evaluation Method

The overall method of evaluation did not change from the first institute in 2014. As described in [8, 13], students were given surveys to fill out by the external evaluators before attending the institute (“pre-survey”), at the end of each day of instruction before the evening lab (“daily surveys”), and after the conclusion of the institute (“post-survey”). We incorporated a scheduled “survey time” each day so that students would be more likely to fill out

²In 2014 this ratio was 5:1; it increased in 2015 due to a large class size with more XSEDE students participating and that being the first year additional guest students were invited to attend.

the daily survey, and the response rate was 90%. Although the pre- and post-surveys were taken by the students off-site, there was a high response rate for these as well: 88% for the pre-survey and 80% for the post-survey. Both the BWSIP and EMPOWER programs required that students complete these surveys, likely contributing to the high response rate. The external evaluation group chose approximately two-thirds of the students to attend private focus group sessions during each institute where they were asked to comment on their experiences up to that point in the institute. By analyzing the results of these evaluations, the instructors were able to assess impact and make informed adjustments to the curriculum in subsequent years.

3.2 Impact of Institute

Throughout the years since participating in the institute, numerous students have gone on to graduate school or work in research environments (sometimes both), with many crediting the institute in helping them achieve their successes. Many of these students belong to groups underrepresented in STEM and HPC.

Colleen Heinemann, student from the 2014 institute, said, “I firmly believe I would not be where I am today without the Blue Waters Institute. I can say without a doubt that the Blue Waters Institute is where I discovered that a career in HPC and scientific visualization was exactly what I wanted to be doing. [...] The information was presented so clearly and effectively that after participating in the institute I had the skills and knowledge necessary to be invited back as an instructor for the institute every year since I was a student” [12]. Heinemann is now a PhD student at UIUC and has worked with the visualization group at the Lawrence Berkeley National Laboratory since completing her undergraduate degree.

In addition to helping students learn programming and computational thinking skills, the institute gave the students the confidence to pass such skills on to others. As said by Caroline MacDonald, student from the 2017 institute, “The Blue Waters Institute was extremely beneficial to me, not only for my past undergraduate research, but for my current graduate school studies and teaching positions. [...] The [Geosciences] department felt that I was qualified to teach [Computer Methods in Meteorology] because of my prior coding experiences and successes, one of which being my participation in the Blue Waters Institute during the summer of 2017. [...] This institute has made me confident that I am able to aid and teach undergraduate students about different programming languages and visualization products” [16]. MacDonald is now a Masters student and Teaching Assistant in Geosciences at Mississippi State University.

While many of the students were from Research I institutions (R1, “very high research activity” according to the Carnegie Classifications [6]), each year we had a number of students from institutions with a lower level of research activity. We also had students from institutions focused on teaching rather than research. These included “baccalaureate colleges”, “masters colleges”, and doctoral Research II (R2) institutions. For these students, access to HPC resources and education would otherwise be difficult or impossible to obtain, and the institute presented an effective way of learning concepts early in their academic careers without having to wait to go to graduate school or enter the workforce to learn them. Dr. Xinlian Liu from

Hood College, a small liberal arts school, mentioned that his intern Thomas Corcoran (2016) went on to an internship at Lawrence Berkeley National Laboratory and said, “[The institute] is a unique opportunity for a small college as we are in. It enabled us to offer an opportunity to our students to get exposed to science and make a serious contribution” [15]. The institute also enabled academic and professional networking opportunities for students at smaller institutions; as Bryton Anderson (2018) from Boise State University (doctoral R2) said, “The institute opened many doors for me, including the opportunity to go to the Supercomputing Conference in Dallas, Texas in November of 2018 as a student volunteer. While at the conference, I was able to network with the national labs, Nvidia, Cray, as well as many others.” [2]

The institute also made a lasting impact when it came to providing students with the ability to produce top-notch research outcomes of publishable quality. For example, approximately 24% of the Blue Waters interns published student papers in the Journal of Computational Science Education (JOCSE). Numerous students published additional papers in journals such as the Journal of Physical Chemistry and presented posters at conferences such as the Blue Waters Symposium series, the Practice and Experience in Advanced Research Computing (PEARC) conference series, and the Supercomputing conference series. To date, institute students have produced at least 50 publications and 63 presentations based on the research projects on which they immediately started working after participating in the institute. Some projects are still ongoing, and additional publications and presentations are anticipated.

In October 2018 we did a survey of the 2014–2017 Blue Waters interns’ LinkedIn profiles to gather data about their current professional statuses. Of 59 students for whom we were able to find these data (79% of the total number of students), 22 were in graduate programs, 18 in industry, 12 still in undergraduate programs, 3 in education, 2 in government, 1 academic staff, and 1 in law school.

4 ASSESSMENT-DRIVEN CURRICULUM DEVELOPMENT

Much of the curriculum development process for the initial 2014 institute is described in [13]. Since then, numerous enhancements and modifications were made daily based on formative (day-to-day) assessment and yearly based on summative (outcome-driven) assessment. Additionally, adjustments were made to tailor the curriculum to the backgrounds of current students and to keep up with emerging topics and trends in the field.

Students responded to daily surveys that helped inform the instructors on adjustments to make as the institute progressed. Figure 5 shows averaged intern responses to the statement, “There was an appropriate balance between lecture and hands-on experience”. In the first few years of the institute, some of the core sessions were deemed to be too lecture-oriented, leading the instructors to modify the curriculum to break up long lectures with practical activities to keep students engaged. Depending on the student pool and development of the curricular materials each year, some activities were deemed to be too focused on lecture or too focused on hands-on exploration. The OpenMP topic shown in Figure 5 is an example of fluctuating scores for the balance between lecture and hands-on

Figure 5: Students’ feedback (averaged) on hands-on versus lecture balance for some of the core topics from 2014 to 2018 (number of responses for any given topic in any given year ranged from 16 to 24). The topics listed on the x-axis were presented, in general, in sequence from one day to the next. The interns were asked to respond to the statement, “There was an appropriate balance between lecture and hands-on experience” with 1 (Strongly disagree), 2 (Disagree), 3 (Neutral), 4 (Agree), or 5 (Strongly agree).

year to year. In 2017, students said that there was too much lecturing, while in 2018, following our adjustments, students said there was too much hands-on practice and not enough guided lecture. By immediately consulting the end-of-day survey data for the OpenMP topic in 2017, the instructors noticed the student feedback concerning too much lecturing and quickly re-balanced the MPI material for the next day to include more hands-on activities. Similarly in 2018, where the opposite sentiment of hands-on vs. lecture balance was found, the instructors provided additional lecture to supplement the hands-on activities. In both years, the adjustments led to an increase in the score for the MPI topic relative to the OpenMP topic of 16% in 2017 and 52% in 2018.

The instructional team made other changes over the years to improve the educational experience based on suggestions from the external evaluation team. For example, following the 2014 institute, the external evaluation team reflected, “Since some of the participants had no computer science background, it was not easy for them to follow all the new knowledge being presented every day.” [7]. Students also commented they felt overwhelmed by different example programs in each session, requiring them to simultaneously try to understand both the program and the concepts being introduced in that session. Based on this feedback, we decided in 2015 to use a single example program for almost all sessions, calculating an approximate value of π using area under a curve. Using a single program allowed the students to work to understand the program once and then concentrate on learning new HPC concepts with that program as a basis.

Although the π example helped students in 2015 not to feel overwhelmed by multiple programs, we also received feedback

after the institute that some students were not sure how to apply the concepts they learned to other programs they came across that were not sufficiently similar to the π program. To address this issue, in 2016 we identified existing—or developed new—science-based examples we could use that would be simple enough to understand quickly but also similar enough to other programs students might encounter in their research.

For example, we used “GalaxSee,” an N-body gravitational model [14], “Pandemic,” an agent-based model of a spread of a disease [19], a forest fire model [22], and a model of heat diffusion [21]. A key design feature was that we made sure the examples we gave to students were already coded, rather than having students start with a blank page and code the programs themselves from scratch. By using pre-coded examples that already worked, we were able to demonstrate to the students how the HPC concepts functioned and were implemented in a working, science-driven example that they could understand without a large amount of cognitive effort.

We also added a session at the beginning of the 2016 institute introducing the C programming language, since it was the foundation for nearly all of the example codes that were provided to the students, and many students entered the institute with only a basic grasp of C. The effectiveness of these changes was reflected in the feedback we received; for instance, one student commented in a daily survey: “Aaron’s fire and heat codes were really well written [...] I will definitely be keeping them for reference - for both OpenMP and generally C tips” [7].

Another area of improvement driven by student feedback was the dissemination of source code for lesson examples. While early years of the institute had students download files from Shodor’s in-house

content management system, in later years the instructors set up a GitHub [10] account (for instance, lead instructor Aaron Weeden's account [20]) so students would have practice using the Git [9] "version control" system for their own projects. Version control is an important concept for those involved in using or producing scientific software, as it provides a mechanism to synchronize the work of multiple developers, keep track of changes to the software, record a log of reasons for those changes, and roll back changes to a particular point in time. Using a version control system for the institute was particularly helpful when students uncovered bugs in the code used in a session: fixing the problem was as simple as uploading a patch to GitHub and having the students download the patch to their laptop. In the 2018 institute, to emphasize the importance of version control, the instructors taught the basics of Git at the beginning of the institute, instead of the end as was done in previous years. Subsequent sessions could then reinforce the techniques required to use version control, rather than have it seem like an ancillary topic at the end of the institute.

5 FUTURE WORK

With approximately 40 hours of core instruction coupled with 20 hours of labs and another 20 hours of additional instruction, the amount of instruction time comprising the institute is nearly as much as a pair of semester-long college courses, or a single semester-long course with a lab section. After five years of development, we have a large pool of lessons, example codes, and other resources that can be drawn upon. The instructors plan to formally adapt the institute curriculum into a course with modular lessons that can be included in an "à la carte" fashion. Part of this work will involve employing more formal instructional design techniques than we have used to date, for example Bloom's Revised Taxonomy [3] for assigning learning objectives to each lesson. This will require collaboration with instructors in various disciplines and institutions in the formal adoption and assessment of the curriculum in their own classes, including collecting feedback and suggested improvements to the curriculum that can be incorporated in the future.

An additional step will be to secure funding for future iterations of the institute, this time inviting faculty to participate in addition to students, thereby "training the trainers" by demonstrating how to deliver the curriculum in a live class, with the expectation that the faculty will return to their own classes and reach even more students. We will also review similar curriculum development efforts from recent years, such as The Carpentries [5], which will help us adapt our curriculum based on lessons learned from others' efforts.

6 CONCLUSION

The goal of the Blue Waters Petascale Institute was to provide a diverse group of students who did not necessarily have parallel programming or HPC experience—or even the opportunity to gain this experience—with the tools and knowledge necessary to complete year-long research projects within their respective disciplines or fields of interest. Results show that, overall, students considered the institute a positive experience and felt they gained the confidence and knowledge necessary to be successful in their internships and beyond in their careers. The institute helped propel students into

graduate programs and the HPC workforce, and it stimulated their production of high-quality research publications and presentations. The continued development of the institute through formative and summative assessments contributed to the development of a broad and diverse HPC workforce.

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