Challenges and Accomplishments of the Computational Science Undergraduate Research Experiences Program

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ABSTRACT

The Computational Science for Undergraduate Research Experiences (CSURE) is an NSF funded Research Experiences for Undergraduates (REU) program organized by the University of Tennessee's Joint Institute for Computational Sciences (JICS), www.jics.utk.edu/csure-reu. The main goal of the CSURE project is to direct a group of undergraduate students to explore the emergent computational science models and techniques using the supercomputers at the National Institute for Computational Sciences (NICS). In addition, a number of summer interns from Hong Kong also participate in the program. The CSURE program focuses on five different scientific domains: chemistry and material sciences, systems biology, engineering mechanics, atmospheric sciences, and parallel solvers on emergent platforms. The program also enjoys a close affiliation with researchers at the Oak Ridge National Laboratory. Because of these diverse topics of research areas and backgrounds of this project, in this paper we discuss the challenges and resolutions in managing and coordinating the program, delivering cohesive tutorial materials, directing mentorship of individual projects, and lessons learned in the duration of the program.

CCS Concepts

Applied Computing--Education; **Social and Professional Topics—Computing Educations—Computational Science and Engineering Education; Computing Methodologies—Parallel Computing Methodologies**

Keywords

Computational Science; Educational Outreach; Research Experiences for Undergraduates

1. INTRODUCTION

Computational science is an emerging field of study that is truly interdisciplinary, involving researchers from mathematics, computer/information science, and many domain science areas. Computational modeling and simulation have become indispensable tools in nearly every field of science and engineering. The CSURE program gives students a synergetic set of knowledge and skills that are useful for them to perform scientific research on high performance computers (HPC).

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The program focuses on five different scientific domains (Figure 1): chemistry and material sciences, systems biology, engineering mechanics, atmospheric sciences, and parallel solvers on emergent platforms. The program starts with a two-week training session, introducing the students to the supercomputing environment and the common computational methods and tools to be used later. Each student is assigned a project complemented to his/her academics background and computing skill level and solves a computational modeling problem under the supervision of a team of mentors and advisors.

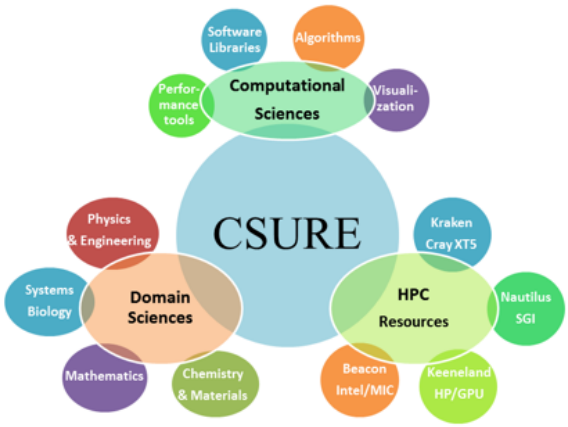

Figure 1: Overview of the CSURE program

From 2013 to 2015, the program has admitted a total of 42 students. Twelve of them are international students from our two collaborating institutes from Hong Kong and three local students are supported under a separate REU grant from other colleges at UTK. The CSURE program has attracted students from 20 different colleges across the nation. Out of the 27 domestic students, 11 are women and 8 are African Americans (2 females). The students worked on a total of 25 different research projects with a total of 16 different lead advisors and 18 mentoring research staff and student associates at the National Institute for Computational Sciences (NICS). The program also enjoys tight collaborations with researchers at the Oak Ridge National Laboratory. Given the scope of activities and size of students and staff in making this program a fruitful experience for the participants, we discuss the challenges and resolutions in managing and coordinating the program, delivering cohesive tutorial materials, directing mentorship of individual projects, and lessons learned through the program. The focus areas and learned lessons are highlighted in bold in the following sections.

2. DESIGN and PLAN

The CSURE program draws from the computational sciences expertise of NICS and the experiences accumulated over a decade from our collaborative summer program for students with the Chinese University of Hong Kong under the direction of Dr. Kwai Wong. The CSURE goal is to promote the ability of undergraduate students to succeed in a research-oriented program in computational sciences. This program presents the participants a good knowledge of how a graduate project is organized and executed. Hence, ***the CSURE program seeks to mimic the pace and intensity of graduate-level or industrial-level projects with well-defined deliverable deadlines.*** In addition, its intellectual focus is not only to push for fruitful research outcomes, but also to expose the students to research experiences through appropriate levels of motivations and accomplishments. These are major reasons we chose to do a ten-week long research program, giving students enough time to master the skills in accomplishing their research goals. While the primary goal of the CSURE REU program is to develop students' interest in pursuing research careers, we also provide strong professional development, post-program development opportunities, and social networking for the REU participants among themselves. Students are encouraged to continue their research activities at their home institutions afterward. There are five major tasks that the students are asked to follow. These tasks start with a preliminary lecture presentation and a poster presentation in the mid session of the program and conclude with an open lecture presentation, a final poster presentation, and a final report in the last week. These tasks aim to gradually assist the students towards finishing their research goals in time. A detailed listing of the CSURE program is available at the webpage, www.jics.utk.edu/csure-reu.

2.1 Schedule of the CSURE Program

For a program as diverse as CSURE to maximize the impact for the participants, a well-planned step-by-step schedule for the entire summer is in place by early December. Event items for the preparation period includes logistical arrangements, program announcement and recruitment, selection of students, payroll registration, identification of research projects and mentoring teams, social activities, preparation of training materials, evaluation instrumentation, mentor selection and training, and the completion of the program agenda. Following that will be the ten-week summer program starting the first week of June and ending the first week of August. A typical daily schedule for the last three years can be found on the CSURE webpage [1]. A typical timeline of the program is listed in the following table.

Table 1: Timeline of the CSURE REU program

Jan. - March	Student recruitment and research project identification
March	Student selection and research project selection
April - May	Prepare training materials, setup research plan, post detailed schedule
May	Mentor training, prepare reference materials, coordinate travel and logistics
First day	CSURE Logistics, campus tour, CSURE goal statement, and survey, Q&A,
1st week	Training and hands-on workshop, meeting mentor, define and formulate research goals and plan of projects
2nd week	Students finalize research plan with mentors, 1st social gathering
2nd – 4th week	Continue research work, PC cluster building
5th week	Preliminary presentation, 2nd social, zoo trip
6th week	Preliminary poster presentation
7th – 9th week	Finishing research work
10th week	Prepare final presentation, final poster, project report,
Last day	Survey, Q&A, retrospective movie, finalize report, summary
August	Summarize results, follow up survey to students and advisors at home institutions
September	Survey report, final report, project continuation
October	Final NSF yearly report submission

The last week of the program is reserved for reporting, presentations, surveys, and meeting with students. It is important to have a detailed check out list for each student and a cordial discussion session with each student. The discussion session involves soliciting general impressions from each student, including upsides and downsides of the program, ideas for improvement, and future opportunities for project work and graduate school. These discussion sessions provide valuable insights to the advancement and improvement of the program.

2.2 Recruitment and student selection

The NSF Computer and Information Science Engineering (CISE) directorate has a joint recruitment program for REU students [2] but the CSURE program opts to do additional recruitment because of the diverse, interdisciplinary nature of the program. CSURE relies on recruitment through emails and contacts with collaborative institutes of NICS and ORNL, particularly with an established outreach partner, Morehouse College in Atlanta. Many of the applicants are highly recommended students through the contacts of our collaborators.

Candidate students considered for this program fill out an application form and write a short essay describing their background, interests in science, and their goals for the program. This information is used to select students and then to assign them to work on the proposed core science domains, to ensure that the specific proposed projects are beneficial to the students matched to their interests, background knowledge, and skills.

Student selection is not always a straightforward process because of the diverse, multidisciplinary nature of this program and the challenge in finding participants that match for the various research topics. A group of mentors meets at least twice to iterate over the applicants, ranking the students for their suitability to the program and the research topics. The deadline for applications is in the middle of February but could be moved back depending the need for more applicants interested in specific research topics.

Participants are selected based on three major factors: the nature of their home colleges, their interests and background, and their letters of intent and references. Students from smaller schools with fewer research opportunities preferred in order to expand the national research community. Rising senior students

are preferred. GPA is a deciding factor only if two candidates have comparable qualifications. Over the course of CSURE, we have not seen that GPA is necessarily predictive of success with the program.

Each summer that are five research topics; generally two students are assigned to work on each research subject. Each pair starts off together but often splits up to work towards separate research aspects of the same topic at the midpoint of the program.

Acceptance letters should be sent out as soon as the first deadline is passed. Getting a written commitment from each accepted student is important. A second set of acceptances is always needed as there are always students declining to attend. Declination letters also need to be sent out in a timely manner; however, it's wise to keep in contact with a few applicants in case of unexpected availability. There are cases that students withdraw late in April for sundry reasons.

2.3 Logistic Support and Research Environment

There are complicating issues for the summer program. The program includes students from a foreign country. It has mentors from UTK and ORNL. The students will have access to supercomputers at NICS. Conference and meeting rooms have to be arranged. Visitor badges must be processed. The students each have separate travel plans. Housing must be arranged. ***All of these issues require timely efforts, coordination, patience, and most importantly, a good support team for a smooth program. Housing for students is the most difficult logistical issue to be resolved and must be prepared early. The entire group should stay together in the arranged housing to help them to blend together socially. It helps to grow a solid bond among the students by organizing group activities and encouraging the students to create their own activities.*** We determine the housing in early February and proceed to place the students as soon as we have finalized the list. We choose to stay in a nearby off-campus apartment complex to significantly cut down the expenses for the students. More importantly, the students are responsible for their own rental agreements.

Reservation of venues for the planned activities such as group photo sessions, lecture presentations, poster presentations, and social gatherings are done early to ensure availability. The group works in two locations, generally two days a week at the University of Tennessee/JICS building at ORNL and the rest of time at the main campus of the University of Tennessee, Knoxville. The location at UTK is a large multi-purpose computing laboratory that can hold 20 more people. It is also used as a lecture and discussion room. There are also a number of student helpers, mostly undergraduate research associates working at JICS, working in the room to answer questions and resolve problems immediately. Co-locating the entire group and student helpers in a multi-purpose room strongly enhances the cohesiveness of the program. There are also classrooms available nearby for private discussions.

The JICS facility represents an investment by the state of Tennessee and features a state-of-the art auditorium, conference rooms, and suites for students and visiting staff. JICS provides the CSURE participants with exposure and access to different leading edge parallel computing platforms (e.g., multicore processors, hybrid systems with GPUs) available at NICS. The JICS mentors include UT faculty, staff members in ORNL research groups, and joint faculty with appointments at both UTK and ORNL. The institute also employs professional research staff, postdoctoral fellows and students, and administrative staff. The CSURE program has benefited tremendously from this infrastructure and staff support.

2.4 Social Activities

The program starts off with a campus walk and a group lunch on the first day. There are also two organized pool gatherings in the apartment complex. The first one is jointly organized with students from another REU program at UTK. They also participate in activities organized for undergraduate summer interns by the UTK office of research. Such activities include a tour of the Neyland football stadium and a few luncheon talks about graduate school application and scholarship information. A hiking trip to the Great Smoky Mountain National Park is arranged. The highlights include a trip to the Knoxville zoo and a tour to the Spallation Neutron Source facility at ORNL. These social activities help to bring the group together and improve morale. ***Importantly, we have arranged a local student to serve as the lead of the group, helping the group to resolve some of the logistic issues in town.***

Having a group of foreign students is a unique element and a contribution of this program. The resulting diversity presents great opportunities for learning about new cultures and different perspectives on computational science research. As the program goes by, the students mix well and enjoy sharing ideas as well as activities such as cooking together.

3. RESEARCH WORK AND MENTORSHIP

The CSURE program addresses the growing importance of computational sciences in many advanced degree programs. The agenda of the proposed program is organized around a synergistic set of ideas and practices that are common to many scientific domains. The focus of the projects leverages the multidisciplinary expertise of the staff in NICS.

In order to provide incoming CSURE students with the most valuable and realistic experience in computational science we have carefully chosen five different areas of significant interest. A CSURE participant is able to select a scientific area in which he/she would like to be involved. Students are paired to work as a team together with their assigned scientific mentors and advisors.

3.1 Training Phase

Student activities include classroom instruction, hands-on exercises, literature search, experimental and modeling design, and computational studies. The program begins with a kick-off meeting to highlight the agenda of the program and introduce the team of researchers and staff working in the project. A tutorial package containing a series of lecture materials and a clear calendar of schedule of work, brown bag lunches, seminars, and activities is published on the CSURE website [1] and is available to the participants.

The first day is reserved for payroll paperwork, initial survey, introduction, exchanging email addresses, Q&A, introducing a local student team leader, and a campus walk. ***A list of safety reminders, health concerns, and emergency contact information is discussed in detail.*** During the program sessions, occasional health issues arise and we once fielded a midnight emergency call to stop a water leak that almost flooded an apartment!

The first week of the program includes an in-depth introduction to the use of supercomputers, including programming languages and compiling procedures, batch queuing systems, and I/O tools. The

materials are drawn from tutorials, specifically including local training materials (e.g., http://www.nics.tennessee.edu/eot/hpc-training) already available from NICS for computational scientists, but adapted to the level of the undergraduate students through feedback and comments from University of Tennessee Knoxville (UTK) undergraduate students. The tutorials come with hands-on exercises that put them to work as a team. Recognizing there is an uneven level of expertise in computing, we always pair the team up to compensate for their knowledge in computer and domain sciences.

An important task of the first week is to assign specific tasks to students to help them begin making progress on their research topic. The project assignments are sent to students ahead of time; however, it is still good to let them know they could possibly change their topics if necessary before the third week of the program. The introductory sessions intersperse lectures with discussion questions, group work on problem solving, and hands-on exercises. Student work on problem solving and hands-on exercises carefully evaluated to determine if any student is having difficulty keeping up, and if further explanations or background may be needed before proceeding to more advanced material.

The second week of the summer includes an introduction to the domain science areas and the specific project content assigned to each team of students. This involves hour-long talks by the subject mentors. We avoid asking students to spend time on learning material that they won't use. In general, only morning sessions have talks, leaving the afternoon session for students to get familiar with the specific software they use or related topics. The rest of the week involves discussing methods for literature search, reading and discussing relevant articles, and hands-on practice with relevant computational methods and tools.

Each student drafts a research plan under the direction of his/her mentor and keeps a weekly research log. Although students may work in groups of two, each will be expected to write a portion of a report describing their research findings and its significance. The students conclude their short plans and a project goal in three weeks. Student progress toward their planned goals is evaluated frequently during the program.

3.2 Research Projects and Mentorship

The research topics available for the CSURE participants span a wide range of scientific and engineering domains. Each of the following areas corresponds to significant capabilities at NICS with active researchers and projects that can be leveraged for the CSURE participant research.

The CSURE topics are chemistry and materials science, systems biology, engineering mechanics, atmospheric sciences, and parallel solvers on emergent platforms. A primary mentor is assigned to each project. Two additional advisors are also assigned to each research team. ***A program director available in a regular basis to lead the overall program is important, particularly in the first half of the program.*** In CSURE Dr. Kwai Wong oversees the program and is always available to participants.

The lead mentors are designated persons committed to the CSURE program. Mentors are selected based on their availability and commitment. They are leading researchers in their domain science working at UTK and/or ORNL. The team of mentors defines the major element of success of the program. They are chosen early and are involved in the selection of students. The student research projects vary every year but fall in the scope of the five program subject areas. In general mentors meet with their students at least twice a week and are available for questions. Graduate students of the mentoring team are in general also available to provide constant guidance and direction to the students. Given the reality that travel for conferences, reviews, or other purposes makes it likely that mentors will occasionally be absent, having additional advisors is important to ensure steady progress. General oversight of the research progress by the program director is also recommended. Regular discussions between the program director and the mentoring team are also helpful.

3.3 Progress Oversight and deliverables

The program has five deliverables. These are designed to steer the students to finish their projects on time. The timeline of these deliverable is listed clearly on the webpage and emphasized in the first week of the program. ***The first deliverable is a preliminary presentation of the research topic and the approach, and is quite important to their success.*** The presentation work orients the students to their work, helps crystallize the approach, and makes students very aware of the project timeline. The program director uses this opportunity to work with the mentors and students to ensure the progress of the research work.

The second deliverable is a poster presentation, organized with three other groups of REU students. The posters help students to organize their first set of results and present them in a public session. Students also have the opportunity to review other projects and potentially seek ideas to improve theirs.

The last two weeks of the program have the students working toward concluding their projects for open presentations. The third and fourth deliverable are similar in nature, one is an open presentation given in the JICS lecture auditorium, and the other is a final poster presentation given at a joint session with over a hundred of summer interns at ORNL. Each presentation lasts for 40 minutes and usually receiving a number of questions from their peers and attendants. The presentations are great experiences for the participants and represent a concluding milestone for their research endeavors.

The last piece of work is a report. This is, in fact, a continuous process, with students organizing their weekly summaries and articulating their results in a detailed report. The students are encouraged to write down a weekly summary report. The final report will be a combined work that documents their progress and their findings. ***Yet in fact, this turns out to be the most demanding part of the 10 weeks experience. Hence it's very important for the program director to keep reminding students throughout the program to work on documenting their efforts and results.***

3.4 Survey

Evaluation of the program is centered on the toolkit distributed by the NSF CISE REU program as published by the University of North Carolina, Charlotte [2]. The evaluation provides the mentoring team with regular feedback for ongoing assessment of the program via in-person meetings along with formal mid-program and annual reports. Reports include evidence-based recommendations for program improvements in the form of clear actions items that program directors can apply directly to further program improvement. A final summative report examines and determines to what extent the program succeeded in meeting its stated goals.

Surveys for the students are performed at the start of the program and at the end of the program. We use the standalone A La Carte student survey from the CISE REU toolkit [2 site]. In order to evaluate the project's impact on participants, students are given pre- and post-evaluation surveys that assess their attitudes toward and interests in computational science, as well as their knowledge of computational science and its use in the domain focus area. The results of these surveys each year guide modifications to the project for future years. Surveys and summative evaluations are independently instrumented either professionally by a contract agency or a person that is familiar with the process. We have done both. In 2015, the REU program engaged Dr. Christian Halloy, a retired computational science leader to conduct the summative program evaluations. Dr. Halloy conducted pre- and post-participant surveys, a personal discussion talk with each participant, and provided a detailed final report. He also attended and critiqued the progress of the students' final lecture and poster presentations.

3.5 Program Outcomes

Over the last three years, we have instituted a multidisciplinary computational sciences REU program that encompasses 25 different projects, including a total of 42 students from 20 colleges, 30 mentoring advisors, 4 full time undergraduate and graduate students, and a team of administrative supporting staff. This program has established a continued relationship with undergraduate institutions for the CSURE program. These institutions include Morehouse College in Atlanta, Maryville College near Knoxville, Centre College in Kentucky, and Alma College in Michigan. This is important in sustaining long-term viability of the CSURE program, which can continue to evolve and improve from listening the feedbacks and suggestions from our partner colleges. The outcomes of the students' research work included six sponsored conference presentations, three conference papers and a number of conference and journal papers to be submitted. A list of their reports is posted in the CSURE website [3]. Over 80% of the students have gone to or are applying for graduate schools. The program director has maintained yearly contacts with the participants. This is important to our sponsor. It helps to track the progress of the students and overall impact to the REU program.

4. CONCLUSIONS

The CSURE program intends to provide participants with an experience with a similar level of effort as in graduate school. The CSURE program provides students an exposure to research with high performance computing applied to a variety of scientific applications. In three summers, we have resolved many problems and met even more challenges. In particular, the following items summarize the highlights of the program:

- *A well-defined step-by-step timeline leading to the end of the program is in place in early December.*
- *The participants are selected based on three major factors: the nature of their home college, their interests and background, and their letters of intent and references.*
- *The project assignments are sent to students ahead of time.*
- *Getting a written commitment from each enrollee is important.*
- *The first deliverable, a preliminary presentation of the research topic and the approaches of the research, is very important.*
- *Housing for students must be prepared in the early stage of the program. The entire group stays together in the arranged housing to get them to blend together socially.*
- *A program director is important, with regular availability to the participants.*
- *Co-locating all students and helpers in a multi-purpose lecturing room enhances the cohesiveness of the program.*
- *A list of safety reminders, health concerns, and emergency contact information is discussed in detail in the first day.*
- *An effective team of mentors represents a major element of success of the program. They are chosen early and are also involved in the selection of their students.*
- *We have arranged a local student to serve as the site lead to the group, particularly for social activities.*
- *Each student begins drafting a research plan under the direction of his/her mentor and keeps a weekly research summary log.*
- *The most demanding part of the 10 weeks experience is the final report. The program director should keep reminding participants and constantly check for progress.*
- *A detailed checkout list for each student and a meeting with each student before the program ends are needed.*
- *Surveys for the students are performed at the start of the program and at the end of the program.*

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