JICS CSURE 2015 Project Report

An NSF Research Experiences for Undergraduates

June 1 - August 7, 2015

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CSURE 2015
An NSF REU Project Report

Overview

The **Computational Science for Undergraduate Research Experiences 2015** (CSURE) is an NSF funded Research Experiences for Undergraduates (REU) program organized by the Joint Institute for Computational Sciences (JICS). The program was instantiated for its first year, during the summer of 2013 on the University of Tennessee, Knoxville (UT) Knoxville campus and Oak Ridge National Laboratory (ORNL). The third year of the CSURE REU extended from June 1 until August 7, 2015. Nine undergraduates were chosen from different colleges in the USA to participate in the CSURE 2015 program.

During the ten-week program, participants lived on an apartment complex near campus at UT, and worked in teams with UT and ORNL research scientists to conduct research in several disciplines requiring computational science tools. The award included a stipend, housing and some funding to support travel for each participant.

PROJECT SUMMARY:

The main goal of the CSURE project is to direct a group of undergraduate students to explore the emergent computational science models and techniques proven to work in a number of data and compute intensive applications using the supercomputers at the National Institute for Computational Sciences (NICS) located at the Oak Ridge National Laboratory. NICS is an NSF funded program managed by the Joint Institute for Computational Sciences (JICS).

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 will give students a synergetic set of knowledge and skills they need to begin using computational methods, as well as provide each student an intensive research experience with a faculty or laboratory mentor.

The 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 for each summer will start with a two-week intensive introduction to the supercomputing environment and the computational methods and tools in the focus areas selected for that summer. Each pair of students will then be assigned a project appropriate for their backgrounds and skill levels in which they will solve a computational modeling problem under the supervision of a team of mentors and advisors. Activities will include meetings and discussions with project personnel, including graduate students and JICS undergraduate interns, group presentations and feedback sessions, attendance at research seminars, and a final report and public presentation.

The five research areas of the CSURE 2015 program

- Chemistry and Materials Sciences
- Computing in Biology
- Engineering Mechanics
- Atmospheric Science
- Parallel Solvers and Emergent Platforms

The CSURE 2015 Program Staff

Principal Investigator (PI): Dr. Gregory Peterson (NICS)
Co-PI: Dr. Kwai Wong (JICS)
Evaluator : Dr. Christian Halloy

Mentors, Trainers and Collaborators:

Allen Jerry Baker, faculty, UTK
Terrie Cassidy, travel Support, JICS, UTK
Angie Chance, secretary and logistical support, JICS, UTK
Eduardo D'Azevedo, research Staff, ORNL
John Drake, faculty, UTK
Joshua Fu, faculty, UTK/ORNL
Scott Gibson, writer, cameraman and photographer, JICS
Christian Halloy, program evaluator
Jacek Jakowski, research scientist, JICS
Yunqi Jin, research scientist, JICS
Srdjan Simunovic, ORNL, UTK
Aleksandar Dimitrovski, research staff, ORNL
Ohannes Karakashian, faculty, UTK
Chung Wa Ng, faculty, Morehouse College
Pragnesh Patel, research scientist, JICS
Dali Wang, research staff, ORNL, UTK
Jacob Pollack, undergraduate intern, REU student, UTK
Patti Redd, User Support Consultant, JICS, UTK
Benjamin Ramsey, undergraduate intern, UTK
Scott Simmerman, research scientist, JICS, UTK
Ying Wai Li, research staff, ORNL
Shiquan Su, research scientist, JICS
Hong Kuo, research staff, Chinese University of Hong Kong
Jun Fan, faculty, City University of Hong Kong
Zhirong Bao, research staff, Sloan Kettering Cancer Center
Xiaolin Cheng, research staff, ORNL
Xiaopeng Zhao, faculty, UTK
Jianhui Tian, research staff, ORNL

Schools Represented at CSURE This Summer

- Central College, IA
- City University of Hong Kong, Hong Kong
- Chinese University of Hong Kong, Hong Kong
- Alma College, MI
- Maryville College, TN
- Morehouse College, GA
- University of South Carolina, SC
- University of North Carolina, Ashville, NC
- University of Tennessee, Knoxville, TN

Scientific Research Projects

Participants were selected to work on one of five research areas: chemistry and materials sciences, systems biology, engineering mechanics, atmospheric sciences, and parallel solvers on emergent platforms. The mentors of these projects have provided a description for each of the projects, and shown in the following pages.

Chemistry and Materials Sciences

Computational chemistry can be used to describe the structure and behavior of matter at atomic scales and often provide essential information leading to new discoveries or enabling better understanding in such diverse fields as drug design, combustion processes, biochemical reactions, and advanced materials design. In the pursuit of sustainable energy technologies, the key to archive an efficient transformation of energy to a chemical form or from one chemical form into another is the presence of suitable catalysts, and the computational study of catalysis will be a primary topic for study by CSURE students. Students will employ a variety of computational techniques including classical dynamics with both classical and quantum-mechanical force fields, density functional theory, and computationally expensive many-body methods made feasible through the use of supercomputers.

Computing in Biology

Due to the revolutionary advancements of next generation sequencing technologies as well as biological research using modeling data, a number of computing tools are utilized to conduct biological simulations. However, data analysis becomes increasingly difficult and can be prohibitive, as existing bioinformatics tools developed in the past decades were developed on computer systems with limited capabilities. Improving the performance and scalability of such tools is critical to transforming ever-growing raw data into biological knowledge that contains invaluable information directly related to human health. This research will help bridge the gap and ability to rapidly analyze data at a large scale, giving a significant, direct impact on science achieved by JICS researchers and collaborators who are currently using these tools on the JICS supercomputer.

Engineering Mechanics

Engineers have been using supercomputers to analyze and resolve many challenging engineering problems for many years. Nowadays, numerical engineering simulation has become a mandatory platform in the process of design and development of many industrial applications from building a mission critical nuclear reactor to manufacturing ordinary domestic products. Often in many of these applications, the material, electrical, thermal, fluid, and structural behaviors of a simulated object are commonly sought. The multi-disciplinary nature of these simulations continues to challenge the engineers and draw interests in the academic research communities.

Atmospheric Sciences

Climate change, weather forecasting, and storm tracking are some of the daunting challenges for ensuring short and long-term safety, quality of life, and environmental sustainability. High performance computing has played a leading role in resolving some of the answers and will continue to do so, and researchers at UT and ORNL are at the forefront of these activities. Research areas that CSURE students have the opportunity to explore include climatic changes, environmental impact assessments, air pollution modeling, the impact of extreme events on health, the impact of transportation planning and energy usages on air quality, the impact of land use (satellite applications) and emissions, diesel track emission effects, energy optimization planning, and numerical model of chemical transport.

Parallel Solvers on Emergent Platforms

An accelerating computing unit, such as Graphics Processing Unit (GPU) or Many Integrated Core (MIC), uses relatively new programming paradigm for high-performance computing applications. There are several advantages of using these units in large-scale supercomputers: (i) They are readily available and inexpensive even in consumer grade video cards; (ii) They offer massive amount of parallelism and high performance, especially for dense matrix computations, (iii) They are significantly more energy efficient than the current generation of multi-core processors. There are many supercomputers in the Top 500 list that are currently equipped with these co-processor units. The new Titan supercomputer at Oak Ridge Leadership Computing Facility (OLCF) at ORNL and beacon in NICS are equipped with accelerators from Nvidia and Intel. However, data transfers between GPU/MIC and CPU are costly and large amounts of parallelism are required to effectively use them. This requires significant retooling or modification of current algorithms such as linear solvers for large dense or structured matrices. The CSURE students have the opportunities to work with researchers at UTK and ORNL on testing and using distributed memory parallel solvers such as PLASMA, ScaLAPACK, and MAGMA that minimize the amount of data movement between processor nodes and between CPU and GPU/MIC.

CSURE Selection Process

There were fourteen participants in the CSURE-REU 2015 program. Nine of these were selected. One additional student also participated but supported by the REU program under Dr. Xiaoping Zhao of the University of Tennessee. Two students from the Mathematics Department at the Chinese University of Hong Kong and two other students from the Physics Department of the City University of Hong Kong also participated in the program. These students from Hong Kong were supported by an educational grant from the Hong Kong Research Council. Each applicant submitted his/her application, which included a goal statement, a CV, his/her transcripts, and two letters of reference. The students were chosen based on the needed basis of their backgrounds, academics seniority, and ability to work with computers. The goal was to gather a diverse group of students that showcased the spectrum of research interests represented in the CSURE-REU program. A panel of mentors gathered at the review meeting and matched up the students to the projects that the students had shown interests in. At the end, the group of 10 American students in 2015 had 3 females, 2 African-Americans and 1 Asian-American (a female) meeting the mandate of the REU program. There were two female students from Hong Kong. The students came from colleges in GA (2), IA, MI (2), NC, SC, TN (3), and Hong Kong (4).

Mentor Training

Mentor training materials was organized and conveyed to each mentor with personal meeting session with Dr. Kwai Wong in May to orientate the mentors about the scope and goals of the CSURE-REU program. Each conference session articulated the importance of the exploratory and training nature of this student research program. During the meeting, we exchanged some of the concerns and potential problems that might appear because of the diversity of the students' backgrounds, sickness, unanticipated vacation requests, office hour accessibility, various levels of mentoring, difficulties of abiding to the defined research program, and lessons learned from last year program. Positive feedbacks were gathered and reflected to the entire mentoring team.

Student Training Program

The training program was composed of two separate sessions. The first session occupied the first week aimed to introduce the goals and nature of the CSURE REU program. Basic knowledge in computing and operation in Linux OS platform were introduced. The mentors in every project topic gave an overview presentation of their work. A rundown of the students' schedule and assignments were also explained. The students would work with their mentors for a week and came back for the second session of training in the third week. The second training session tended to be more interactive in answering and reflecting some of the knowledge that they had encountered in the first two weeks of the REU program. A few more sets of in-depth materials in parallel computing and visualization tools were also introduced.

Abstracts of Student Projects

Atmospheric Sciences

Parallel Discontinuous Galerkin Method for Chemical Transport Modeling - Yin Ki (Kiki) Ng (Mentors : O. Karakashian, K. Wong, Joshua Fu, J. Drake)

Climate and chemical transport modeling on a globe requires the use of unstructured grids, as well as conservation of mass and energy for a stable and accurate simulation. Chemical transport is often simulated using the finite volume method (FVM), which is explicitly conservative. This project explored the fundamental computing framework using discontinuous Galerkin finite element method, which is known a locally conservative method. Due to the interplay between chemical pollution and climate behavior, it is desirable for the formulation of both climate and chemical transport to be based on the same method. The DGFEM for a Poisson problem is used as a test example using both a serial and a parallel code and then will be extended to cover the chemical transport formulations.

Chemistry and Materials Sciences

Modeling of a Graphene Membrane Rupture with DFTB and Improving its Computational Efficiency - Krystle Reiss and Jacob Blazejewski (Mentors: Jacek Jakowski, K. Wong)
DFTB+ is being used to determine the cause of a graphene membrane rupture under the influence of an electric field.[1] When an electric field of 3 V/nm is applied to a graphene membrane suspended in a 1 M KCl solution, the membrane ruptures catastrophically, sometimes ripping completely in half. Several different variations of graphene membranes are being tested under varying conditions using molecular dynamics (MD) simulations. Unfortunately running these DFTB calculations is extremely computationally expensive, with the most demanding calculations being linear algebra operations. The time spent on these operations is divided amongst evaluating forces, determining electronic structure and moving and handling the matrices to be used in the operations. The DFTB code utilizes Linear Algebra Package (LAPACK) functions to perform these calculations. Under these routines DFTB calculations of certain systems can still take far to long to be practical. In an attempt to speed up the software's calculations the LAPACK routines are therefore being replaced with Scalable LAPACK (ScaLAPACK) routines.

Molecular Dynamics Simulation of Melittin in a Dimyristoylphosphatidylcholine (DMPC) Bilayer Membrane - Huanbo Jiang and Zhiyao Xie (Mentors: X. Cheng, J. Fan, K. Wong)

Melitin is the major protein component of the bee venom that has a pronounced effect on the lysis of membranes. The amino-terminal region is predominantly hydrophobic whereas the Carboxy-terminal region is hydrophilic due to the presence of a stretch of positively charged amino acids. This amphiphilic property of Melittin makes it is water soluble and yet it spontaneously associates with natural and artificial membranes.

Molecular dynamics (MD) trajectories of Melittin inserted into DMPC bilayer membrane are generated using MD simulation for a better understanding of protein-membrane interactions, especially interactions involved in the anchoring and stabilization of membrane-bound proteins. Four different systems were constructed. Temperature scan was adopted for DMPC only system and DMPC+Melittin system for phase transition comparison and the effects Melittin and Cholesterol have on the dynamics of DMPC at both liquid and gel phases were observed by measuring some properties of our systems, area per lipid, order parameter, gauche fraction and RMSF value, for instance. Some relative experimental results were also provided here to verify our simulation trajectories.

Engineering Mechanics

Power System Transient Stability Analysis – Ashely Cliff (Mentors: Srdjan Simunovic, Aleksandar Dimitrovski, Kwai Wong)

Electricity is an intrinsic part of modern culture, and having reliable access is a necessity. Power supply systems, i.e. power grids, have the responsibility to produce and distribute steady power to all consumers. Due to the nature of power, and of alternating currents, slight disturbances can cause large amounts of fluctuation and damage quickly. These can cause power outages that can range in severity from a single downed line to an entire country or more without power. The purpose of this project is to create accurate simulations of power outages that can be used to avoid actual power failures. For the simulations to be useful, they must be able to run faster than real time, to determine what will happen when there's an outage before the outcome occurs. To accomplish this, the Parareal in Time Algorithm is being implemented to increase speed up and aid in a logical way to parallelize the code.

Parallel Cardiac Model Simulation – Jacob Pollack (Mentors: X. Zhao K. Wong)

Cardiovascular diseases are the leading cause of death worldwide. Using computer simulations to accurately model the dynamics of the heart provides a platform for developing methods to better detect and treat heart disease. We present a heart electrophysiology modeling framework designed to run on HPC platforms. The model is capable of simulating the generation and propagation of electrical signals throughout the heart under a variety of circumstances.

The action potential of each simulated cell can be described using a variety of different models. However, prior implementations of the cardiac modeling framework only supported the use of the Beeler-Reuter model. Our work refactoring the cardiac model allows the model to be extended to a multitude of electrical model, including the O'Hara-Rudy model [3]. This expansion of functionality dramatically increases the simulation's usefulness, as many applications require the use of novel or complex electrical models. The usefulness and functionality of the cardiac model is expanded via integration with the Distributive Interoperable Executive Library (openDIEL), a multiphysics modeling suite, using various heart meshes and electrical models. The openDIEL provides expanded functionality and allows for other simulations to be run in parallel with relative ease.

Numerical Libraries on Emergent Platforms

Exploring QR factorization on GPU for Quantum Monte Carlo Simulation; Tyler McDaniel and Ming Wong (Mentors: E. D'Azevedo, Y. W. Li, K. Wong)

QMCPACK is open-source scientific software designed to perform Quantum Monte Carlo simulations, which are first principles methods for determining the properties of the electronic structure of atoms, molecules, and solids. One major objective is finding the ground state for a physical system. This project investigates possible alternatives to the existing method in QMCPACK such as QR factorization for evaluating single-particle updates to a system's electron configuration by improving the computational efficiency and numerical stability of the algorithms. The current implementation in QMCPACK for this procedure uses LU decomposition on the matrix A and its extension using the Sherman-Morrison formulation to update the matrix. The scope of the project is to explore updating the matrix using QR factorization and implementation on the GPU System on Beacon, a cluster with Intel Phi co-processor and GPU at the National institute for Computational Sciences (NICS).

Workflow and Direct Communication in the Open Distributive Interoperable Executive Library : Nick Moran and Tanner Curren (Mentors: K. Wong, P. Patel)

The Distributive Interoperable Executive Library (DIEL) is a software framework designed to configure and execute a series of loosely coupled scientific modules in parallel. The DIEL is capable of running many existing users' codes on high performance computing machines such as Darter and Beacon. It includes an interface for inter-process communication that is controlled via a simple configuration file. Currently provided are direct data exchange using user-defined shared boundary conditions and a prototype of indirect data exchange via a global tuple space. The goal of this project is to improve and extend the direct and tuple space implementation to make it a viable and efficient method of communication.

A Multi-Objective Stochastic Programming Model for Disaster Relief Logistics Under Uncertainty ; Helsa Chan (Mentors: Hong Kuo, K. Wong)

Every year, natural disasters including earthquakes, drought, flood and tropical cyclone kill thousands of people and cause large-scale destruction to habitats which often results in a loss of millions of dollars of assets. A well-designed disaster relief management system aids affected people and allows reconstruction at the affected areas in the most efficient way, while an inappropriate allocation of resources results in higher unnecessary costs, supply shortage and increased suffering. Thus, a sophisticated disaster relief management system developed in the pre-disaster stage is highly useful in reducing costs and maximizing efficiency in saving lives. However, the huge complexity and dynamics involved in disasters naturally implies a high level of uncertainty in disaster relief management. Two main features of the problems that a disaster relief planner would face include conflicting objectives, such as minimizing costs while maximizing satisfaction in affected areas, and the lack of knowledge of data, such as demand, supply and cost. Bozorgi-Amiri et al. proposed a stochastic programming model which aims to "model disaster planning and response capturing the inherent uncertainty in demand, supply, and cost resulting from a disaster". Like the model by Bozorgi-Amiri we first formulate our model as a linear programming problem. Then, we build a C program, which integrates a mixed-integer linear programming solver SYMPHONY to find an optimal solution of various case studies. Finally we use multiprocessing to speed up the simulation and solve cases in larger scale.

Computing in Biology

Using High Performance Computing To Model Cellular Embryogenesis – Gerard Vanloo (Mentor: Dali Wang, Z. Bao, B. Ramsey, K. Wong)

Agent Based Visualization of C. Elegans Embryogenesis at Cellular – Kison Osborne, (Mentors: C. Ng, K. Wong. S. Simmerman)

C. Elegans is a primitive multicellular organism (worm) that shares many important biological characteristics that arise as complications within human beings. It begins as a single cell and then undergoes a complex embryogenesis to form a complete animal. Using experimental data, the early stages of life of the cells are simulated by computers. The goal of this project is to use this simulation to compare the embryogenesis stage of *C. Elegans* cells with that of human cells. Since the simulation involves the manipulation of many files and large amounts of data, the power provided by supercomputers and parallel programming is required.

The objective of this project is to replicate the data of the beginning stages (embryogenesis) of a *C. Elegans* worm cell from experimental data through computer simulation. A preliminary version of simulation was done using the agent based simulation software, NetLogo. However, NetLogo is unable to handle large data sets as the software is unable to work in parallel and thus would only be able to perform such a simulation given an impractical amount of time. Thus the simulation has been ported to RepastHPC to solve this issue. A visualization program, VisIt, is used to show to the results of the RepastHPC simulation. This manual will cover only the RepastHPC process. Consult the VisIt manual for instructions for visualizing results from RepastHPC

Initial Stage of the CSURE Project

The CSURE project is a 10-week summer project designed to provide promising undergraduate students experience in the research applications of computational science — and, in the process, get them energized and encouraged about furthering their educations.

Students arrived at the campus of the University of Tennessee, Knoxville on June 1 to start the 2015 program. Through CSURE, students explored the emergent computational models and techniques proven to work in a number of data- and compute-intensive applications. For their assignments, they used supercomputers managed by the National Institute for Computational Sciences (NICS) for NSF and located at Oak Ridge National Laboratory (ORNL). Students competed to be selected for the project by submitting applications containing information about their academic performance and an essay in which they described why they wanted to be a part of CSURE.

The take-away from CSURE will be not only a synergistic set of knowledge and skills to begin using computational methods but also personal growth by way of social and cultural enrichment. The project is composed of 10 (one local student is supported by other REU program) students from the U.S., with an added international element: four students from Hong Kong who are funded by the Chinese University of Hong Kong and the City University of Hong Kong, that have a strong emphasis on research. CSURE students have the opportunity to become well acquainted with one another, because all of them resided in the same off-campus apartment complex for the duration of the project.

In the first two weeks of CSURE, the students settled into their housing, were paired in project teams, met their respective mentors and received an intensive introduction to the supercomputing environment and the computational methods and tools in the focus areas selected for the summer: biology, bioinformatics, materials, chemistry, emergent computer systems, biomedical engineering, climate science and weather forecasting. They also toured the computing facilities at ORNL, including the supercomputer machine room.

Early Activities

On the day of their arrival at UT on June 1st, the CSURE students registered and were then given an overview of their summer internship program, brief project areas and initial selection of the project teams. On the very next day they visited the JICS facilities at ORNL as shown in the picture below.

Participants in the Computational Science for Undergraduates Research Experiences (CSURE) program for 2015, group in left: top row : Ashley Cliff (Center College, IA), Tanner Curren (Maryville College, TN), Ben Ramsey (Undergraduate Intern, UTK), middle row : Helsa Chan (CUHK, HK), Krystle Reiss (Alma College, MI), Front row : Ming Wong (U. of South Carolina, SC), Kiki Ng (CUHK, HK) : group in right : top row : Kison Osborne (Morehouse College, GA), Jacob Blazejewski (Alma College, MI), Nick Moran (UTK, TN), middle row: Gerard Vanloo (Morehouse College, GA), Tyler McDaniel (UNC, Ashville, NC), front row :Bobby Jiang (CityU, HK), Andy Xie (CityU, HK), Jacob Pollack (UTK, TN), not in picture)

CSURE 2015 participants outside at the University of Tennessee and old World Fair site in Downtown Knoxville.

CSURE 2015 participants in the Everest visualization facility and the Spallation Neutron Source facility at the Oak Ridge National Laboratory.

Training on site at UTK and at ORNL:

The first week is also time for the students to become acquainted with their mentors and their projects, which will delve into the domains of atmospheric sciences, chemistry and materials sciences, engineering mechanics, numerical libraries on emergent platforms, and systems biology. The following weeks of the project consisted of in-depth training in parallel programming languages, emergent platforms, general numerical libraries, building a PC cluster and basic networking, visualization, and other applications topics.

The mentoring by high-performance computing (HPC) experts from JICS and the students' pursuit of individual projects, combined with timely and targeted lectures on HPC and leading-edge research in HPC-supported scientific domains are integral to the essence of CSURE: providing the student participants with a synergistic set of knowledge and skills they will need to begin using computational methods.

CSURE 2015 participants in the training session at the University of Tennessee.

CSURE 2015 participants working at a training room at UTK.

Social Activities:

Although the CSURE students will are busy with their project work—which will entail writing a paper, developing a poster, and sharpening their communications skills through one-on-one interaction at poster sessions and audience engagement during formal presentations—they will have opportunities to get to know one another in more relaxed social gatherings and enjoy the beauty of East Tennessee. Among the activities planned are a pool party and outings to the Smoky Mountains and the Knoxville Zoo organized by UT-Knoxville's National Institute for Mathematical and Biological Synthesis, known as NIMBioS.

While CSURE demands a lot of effort in research projects, it can't, however, be fairly characterized as all work and no play, as the students have attested. The entire group of students has been living in the same "off the beaten path" apartment complex a few miles from the University of Tennessee, Knoxville, campus, and such an arrangement has created the right environment for camaraderie, the students say. They've had a pool party at the complex and have regularly played games and watched many movies together, and the Chinese students have demonstrated for the Americans the art behind the cuisine of their homeland.

The students have also gotten to enjoy some of the unique offerings of East Tennessee, such as the site of the 1982 World's Fair in downtown Knoxville. A pool party was organized. The CSURE participants combined outings with the REU students from the UTK NIMBioS program. Trips to the Knoxville Zoo as well as to the Great Smoky Mountains National Park were also organized.

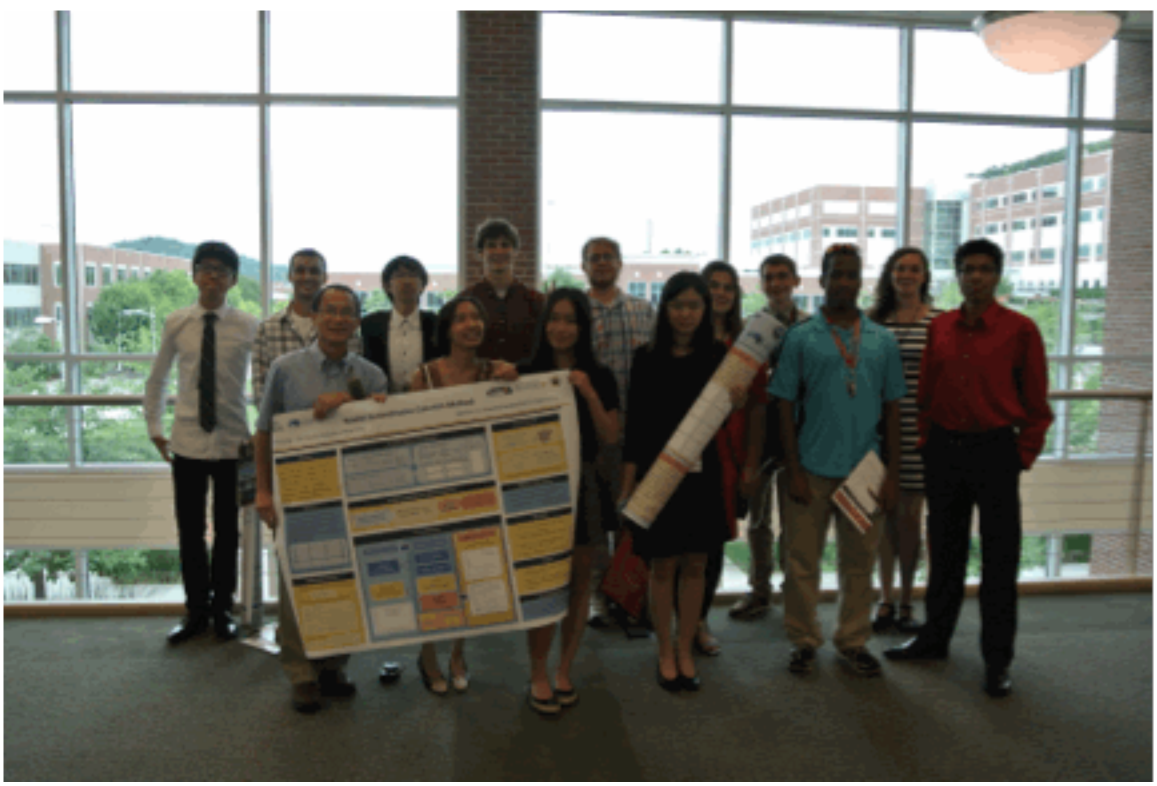
CSURE 2015 visiting the Great Smoky Mountains National Park.

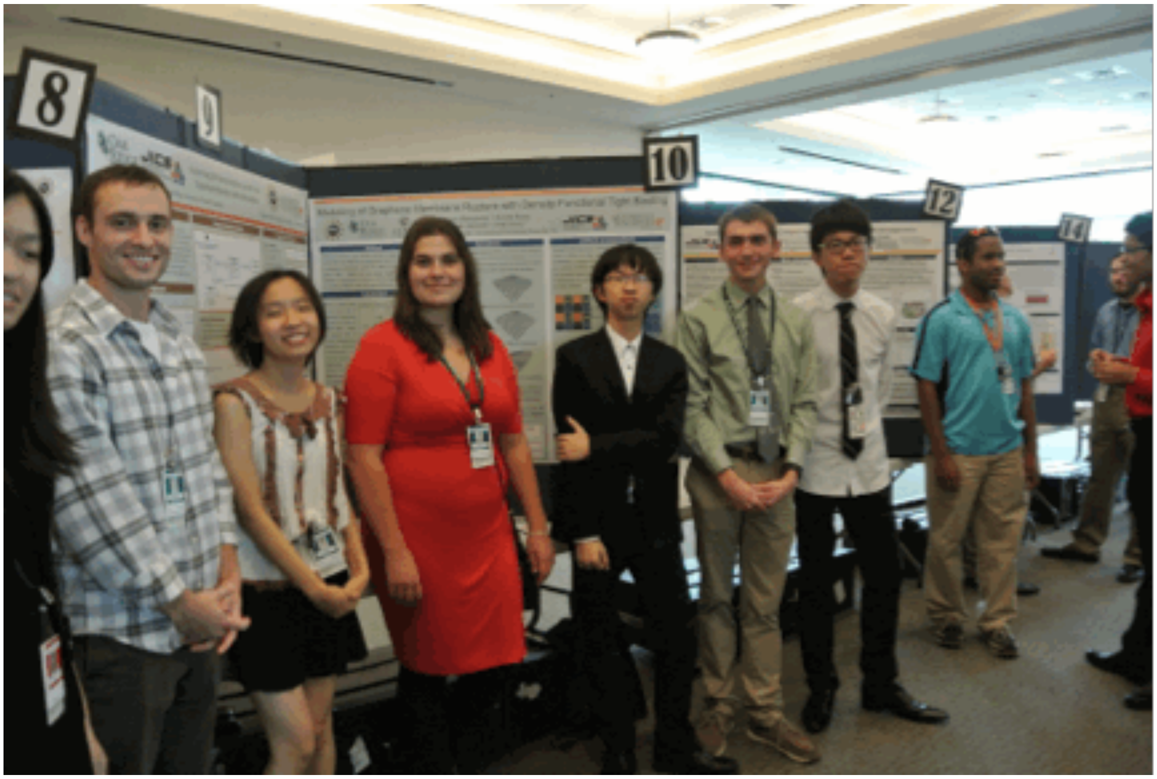
CSURE 2015 visiting the Knoxville zoo.

Poster Sessions and Seminar Presentations:

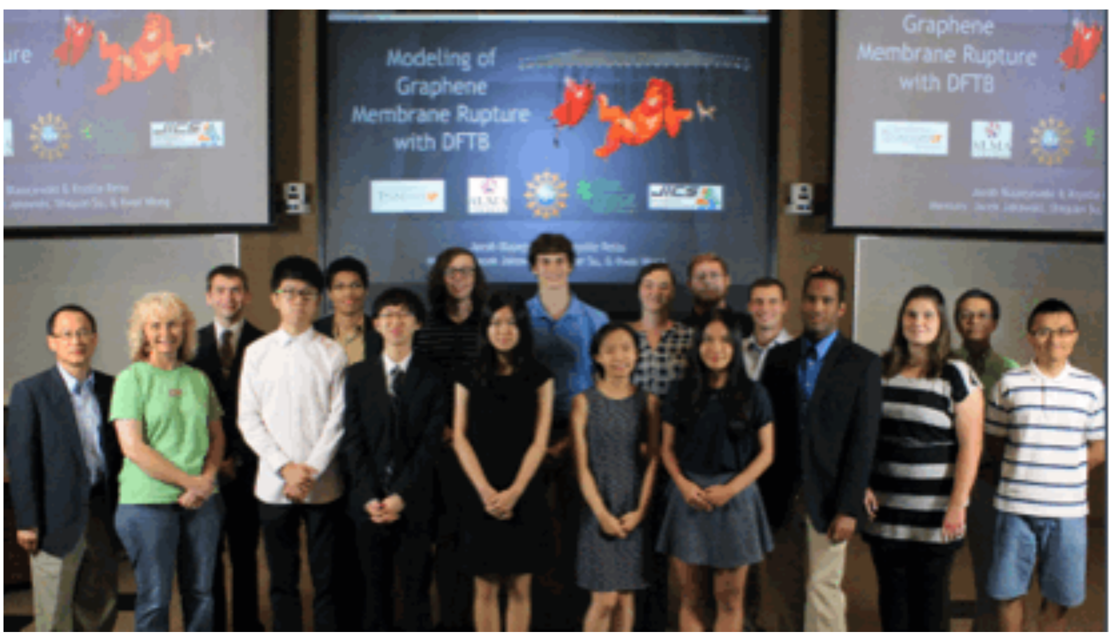
Two poster sessions, one in combination with the NIMBIOS REU program and the other joined together with the interns from ORNL, were held at UTK and ORNL respectively. As the CSURE neared its final week, each participants made an oral presentation during a seminar series and make use of the wonderful auditorium facility in the JICS building.

CSURE participants in their first poster presentations





CSURE participants in their poster presentations at ORNL



CSURE participants and supporting staff and mentors gather for group pictures in the JICS Auditorium after their final presentations

CSURE participants gather for dinner after their program

Conclusions

The Computational Science for Undergraduate Research Experiences (CSURE) summer program concluded its tenth and final week, on August 7th. The comments of the students participating in the program expressed how exposure to the world of research projects and supercomputing with seasoned mentors and other high-performance-computing professionals took their education to a deeper level.

CSURE, presented by the Joint Institute for Computational Sciences (JICS) on June 1–Aug. 7, directed a group of 10 students from colleges and universities across the United States and four from the Chinese University of Hong Kong in the exploration of emergent computational science models and techniques proven to work in a number of data- and compute-intensive applications using the supercomputers at the National Institute for Computational Sciences (NICS) located at Oak Ridge National Laboratory (ORNL). The program focused on five scientific domains: chemistry and materials sciences, systems biology, engineering mechanics, atmospheric sciences and parallel solvers on emergent platforms.

In the first two weeks, the students learned about the supercomputer environment and the computational methods and tools applicable to the focus areas selected for the summer. Each student was assigned a project appropriate for his or her background and skill level to solve a computational modeling problem under the supervision of a team of mentors and advisors. Then, for the duration of the program, the students worked on their projects. Activities consisted of meetings and discussions with project personnel, including graduate students; team presentations and feedback sessions; attending research seminars; and a final report and public presentation.

The design of the CSURE-REU internship program was laid out to reflect some level of similarity of graduate work. The students were asked to do an initial presentation, a mid-term poster, a final presentation, a final poster presentation, and the final report. The level of difficult represented a challenge but it was regarded as a rewarding experience to the students, particularly the ones that were preparing to attend graduate schools.

Overall, the students reflected that the program was hard but appropriately instituted. They enjoyed the process and were amazed that they were able to accomplish the work in time. One of their common comments was that the level of guidance and oversight by the mentors were extremely helpful and crucial to the accomplishments of their works. All their works were documented on the CSURE website, www.jics.utk.edu/csure-reu under the web-link to the program CSURE 2015.

We made improvements to the implementation and mentorship to this year program based on the suggestions and comments from the evaluation of previous two years. There were three poster presentations at the XSEDE meeting and one scheduled talk for the upcoming SIAM LA meeting. The students and their mentors are working on three papers to be submitted in the future.

APPENDIX A: CSURE 2015 Evaluations

Description of the Evaluations

The evaluation of the CSURE 2015 program consisted of two parts: an initial evaluation (or pre-evaluation) performed on the first day of the program (June 1rd) and a final evaluation done on the last day of the program (August 7th). The evaluation of the program was both formative and summative in nature, in that the data collected was intended to both gain feedback from participants about the quality of the current program and also to inform and improve next year's program. A pre/post evaluation design was used to measure self-reported changes in participant skills and knowledge as a result of taking part in the program.

The survey document attached separately to this report, was handled and presented by Dr. Christian Halloy. All students participating in the CSURE were asked to complete a survey designed by the CISE REU Assessment Work group led by Audrey Rorrer at the University of North Carolina, Charlotte before and after the experience. It was obtained from the CISE REU Toolkit (http://reu.uncc.edu/cise-reu-toolkit), using the "A la Carte Student Survey" available at the website, http://reu.uncc.edu/toolkit/la-carte-survey.

Appendix B : CSURE 2015 Detailed Schedule of Planned Activities

First Week : June 1 - June 5

Date	Time	Activity	Location
June 1	9:00 am - noon	Welcome : Check in, surveys, Walk around, computer accounts	Claxton 352
June 1	1:00 pm - 5:00pm	Project assignment, Introduction to Linux and vi	Claxton 352
June 2	8:30 am - noon	Shuttle to ORNL Check, safety list, walk around	ORNL JICS 5100
June 2	1:00 pm - 5:00 pm	Overview of project, meet your mentors at ORNL, Makefile, C, Fortran talk	JICS 5100
June 3	9:00 am - noon	Introduction to Parallel Computing, darter, beacon, rockfrog	Dougherty 406
June 3	1:00 pm - 5:00 pm	Meet your mentor exercises, project work	Dougherty 406
June 4	9:00 am - noon	Introduction to MPI Programming	DO 406
June 4	1:30 pm - 5:00 pm	Exercsies on darter, beacon and rockfrog	DO 406
June 5	9:00 am - noon	Parallel Programming exercise using MPI	ORNL
June 5	1:30 pm - 5:00 pm	Project work	ORNL

Second Week : June 8 - June 12

Date	Time	Activity	Location
June 8	9:00 am - 5:00	Project Science talk I, Project Work	DO 406
June 9	9:00 am - 5:00	Project Science talk II, project work	ORNL
June 10	9:00 am - 5:00	Openmp, openacc, MIC, GPU, Project work	DO 406
June 11	9:00 am - 5:00 pm	PC cluster building using Raspberry Pi	DO 406
June 11	4:00 pm - 9:00pm	Social gathering	Quarry Trail Apartment pool
June 12	9:00 pm - 5:00 pm	Project work	ORNL/DO 406

Third Week : June 15 - June 19

Date	Time	Activity	Location
June 15	9:00 am - noon	Project Work	DO 406
June 15	1:30 pm - 5;00 pm	Project work	DO 406
June 16	9:00 am - noon	Project Work	DO 406
June 16	1:30 am - 5:00 pm	Project work	DO 406
June 17	9:00 am - 5:00 pm	Project work	ORNL
June 18	9:00 am - noon	Project Work	DO 406
June 18	1:30 pm - 5:00 pm	Project Work	DO 406
June 19	9:00 am - noon	Project work	DO 406
June 19	1:30 pm - 5:00 pm	Project work	DO 406
June 19	6:00 pm - 9:00pm	Social Gathering	Quarry Trail Apartment pool
June 20	8:00am	Smoky Mountain Trip	GSMNP

Fourth Week : June 22- June 26

Date	Time	Activity	Location
June 22	9:00 am - 5:00 pm	Visit talk	DO 406
June 23	9:00 am - 5:00 pm	Project work	DO 406
June 24	9:00 am - 5:00 pm	Project work	ORNL

June 25	9:00 am - 5:00 pm	Project work	DO 406
June 26	9:00 pm - 5:00 pm	Project work	DO 406

Fifth Week : June 29- July 3

Date	Time	Activity	Location
June 29	9:00 am - 5:00 pm	Project work	DO 406
June 30	9:00 am - 5:00 pm	Project work	DO 406
July 1	9:00 am - 5:00 pm	Project	ORNL
July 2	9:00 am - 5:00 pm	Project work	DO 406
July 3	9:00 am - 5:00 pm	Holiday	DO 406

Sixth Week : July 6- July 10

Date	Time	Activity	Location
July 6	9:00 am - 5:00 pm	Project discussion : Title for poster presentation	DO 406
July 7	9:00 am - 5:00 pm	Project work	DO 406
July 8	9:00 am - 5:00 pm	Project overview : 3-slide project summary presentation	ORNL JICS RM 262
July 9	9:00 am - 5:00 pm	Project work	DO 406
July 10	9:00 pm - 5:00 pm	Project work	DO 406

Seventh Week : July 13- July 17

Date	Time	Activity	Location
July 13	9:00 am - 5:00 pm	Project discussion with Mentors	DO 406
July 14	9:00 am - 5:00 pm	Zoo Trip	Knoxville Zoo
July 15	9:00 am - 5:00 pm	Project discussion with mentors	ORNL
July 16	9:00 am - 5:00	Project work	DO 406

	pm		
July 17	9:00 pm - 5:00 pm	Project work	DO 406

Eighth Week : July 20- July 24

Date	Time	Activity	Location
July 20	9:00 am - 5:00 pm	Project discussion with Mentors	DO 406
July 21	9:00 am - 5:00 pm	Project work : poster preparation	DO 406
July 22	9:00 am - 5:00 pm	Project work : poster preparation	ORNL
July 23	9:00 am - 5:00 pm	Project work : poster preparation	DO 406
July 24	9:00 pm - 5:00 pm	**Project work : 1st poster : project summary presentation**	UTK

Ninth Week : July 27- July 31

Date	Time	Activity	Location
July 27	9:00 am - 5:00 pm	Project discussion with Mentors	DO 406
July 28	9:00 am - 5:00 pm	Project work	DO 406
July 29	9:00 am - 5:00 pm	Project discussion : final presentation	ORNL
July 30	9:00 am - 5:00 pm	Project work	DO 406
July 31	9:00 pm - 5:00 pm	Project work	DO 406

Tenth Week : August 3- August 7

Date	Time	Activity	Location
Aug. 3	**9:00 am - 5:00 pm**	Project Work	**DO 406**
Aug. 4	9:00 am - 5:00 pm	Project wrap up - continuation program	DO 406 Perkins 317
Aug. 5	**9:00 am - 5:00 pm**	**Final Project presentation JICS auditorium**	**ORNL**
Aug. 5	**9:00 am - 5:00 pm**	**Final Project presentation Due**	**ORNL**

Aug. 6	9:00 am - 5:00 pm	**Final Poster presentation with ORAU summer student , closing program at ORNL**	ORNL 5200
Aug. 7	9:00 pm - 5:00 pm	Closing Remarks : Survey	UTK Claxton