

MCSR Mini-Camp Offers JSU Science Students Computational Foothold

Contributed by Edwin Smith
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Preparing tomorrow's scientists to compute and compete

OXFORD, Miss. - Ten Jackson State University summer students are a little closer to becoming computational scientists, thanks to a recent mini-camp provided by the Mississippi Center for Supercomputing Research at the University of Mississippi.

MCSR hosted the two-day event last week for 12 students attending the Summer Institute at the Interdisciplinary Center for Nanotoxicity at JSU. During the sessions, the students learned how to build and use computational models of chemicals and reactions.

The previous week, MCSR staff members Susan Lukose and Jason Hale visited the JSU campus to lay the technical groundwork for the mini-camp by teaching ICN students the basics of Linux, the operating system used by many of today's supercomputers. This "crash course" was created to give science students a technical foothold in computational research.

Watch slideshow.

"Faculty and student researchers from Jackson State's chemistry department have been major users of MCSR's supercomputers for over a decade," said Hale, manager of research support at MCSR. MCSR and JSU began discussing the idea of creating this opportunity for the Summer Institute students last summer.

"We hope to make this a regular event, and expand the mini-camp into a weeklong training experience for future computational chemists from all over Mississippi," Hale said. Similar training was provided this summer and last for summer research students in UM's Department of Chemistry and Biochemistry, as well as the Department of Medicinal Chemistry.

Shonda Allen, associate director of ICN, said the workshop taught students how to submit computational jobs to the supercomputers and develop advanced skills that will prove useful in ICN's research projects. "As computational chemists, they will be able to conduct research much faster and with less expense than traditional chemists," she said.

"We provided very practical, hands-on training," said Brian Hopkins, MCSR computational scientist who taught the chemistry component of the mini-camp. "Starting with a chemical equation written on the blackboard, they created computer models, ran simulations and came up with accurate computational predictions for various chemical properties and processes."

Besides JSU graduate and undergraduate students, participants hailed from Jim Hill High School, Murrah High School, Hinds Community College, Tougaloo College and Universidad Metropolitana in San Juan, Puerto Rico. All seemed fascinated by the instruction they received.

"Before this workshop I was not familiar with computational chemistry at all," said Don Gibson, a JSU graduate student from Jackson. "Now I can see how a computer can be used to simulate chemical structures in rapid time."

"My career goal is to become a research scientist in molecular chemistry," said Ganna Gryn'ova, a JSU graduate student from the Ukraine. "I can see how what I've learned here will be useful to me in achieving my objective."

Allen said JSU is "most appreciative" for MCSR's initiative in offering both the mini-camp and the brief workshop at JSU the previous week.

"I can tell by the students' responses and the quality of questions they've asked that they are obtaining more usable knowledge," Allen said. "Such skills will greatly enhance their research presentations at both national and international ICN conferences on nanotoxicity."

Since all work and no play can make for a toxic learning environment, the young scientists mixed some fun into their trip as well. On one of the hottest days of the year, they enjoyed a pizza lunch in what might literally be the coolest place on campus - the highly air conditioned Supercomputing Center, where they walked (and had their pictures made) among the giant computers that will crunch their molecular simulations.

Thursday evening, the mini-campers checked out Oxford, where some enjoyed the new "Transformers" movie, and others went bowling. All stayed at the new Inn at Ole Miss overnight Thursday and returned to

Jackson with new MCSR T-shirts after Friday morning's session. Next month, their mini-camp coaches from MCSR will return to Jackson, this time to view the presentations that the JSU students will give to describe their research accomplishments during the Summer Institute, and to present a Linux Netbook computer (donated by Dell) to the student whose summer work demonstrates the most effective use of supercomputing.

Established by the Mississippi Legislature in 1987, the Mississippi Center for Supercomputing Research operates supercomputers for research use throughout Mississippi. MCSR helps scientists at all of Mississippi's public universities compete for and conduct research projects using computational simulation. In FY 2009, more than \$31 million of federally funded research in Mississippi was supported by MCSR supercomputing resources.

Established in 2008, the Interdisciplinary Center for Nanotoxicity, a National Science Foundation Center for Research Excellence in Science and Technology, integrates experimental and computational research with undergraduate and graduate education and training of minority students.

For more information about MCSR, visit <http://www.mcsr.olemiss.edu> .