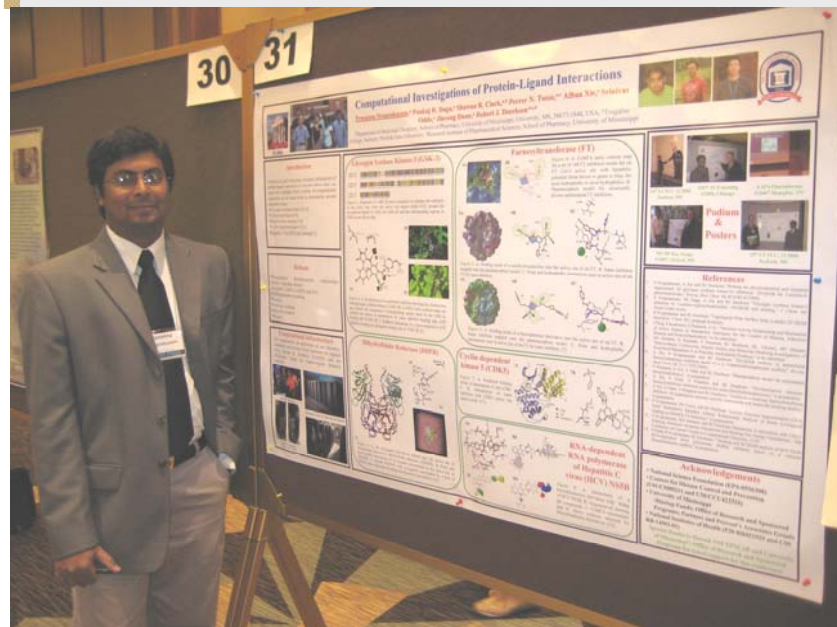
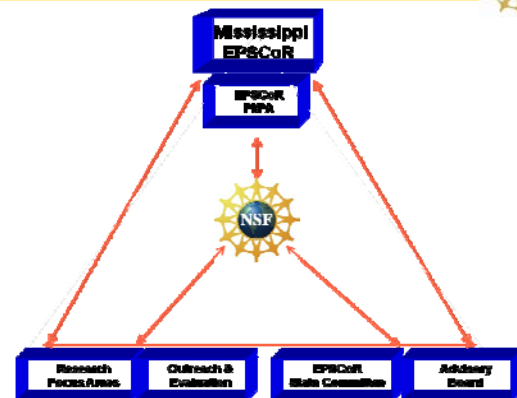




EPSCoR HIGHLIGHT UM student presents research at national EPSCoR Conference



University of Mississippi doctoral student, Prasanna Sivaprakasam, represented the Mississippi EPSCoR team in October when he presented his research titled "Computational Investigations of Protein-Ligand Interactions" at the 2007 National NSF EPSCoR Conference in Hawaii. The theme for the three day conference was "EPSCoR Leadership for Scientific Innovation, Collaboration, and Enculturation." Administered by the University of Hawaii System, university students and faculty had the opportunity to share research being conducted through EPSCoR funding and speak with numerous NSF program officers who were in attendance.



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MISSISSIPPI EPSCoR NEWSLETTER



NSF's Olsen and Barnes to speak at EPSCoR state meeting



Dr. Kathie Olsen, Deputy Director at the National Science Foundation (NSF), will be the keynote speaker during the annual Mississippi EPSCoR meeting this month.

This year's host university will be Mississippi State University. National Advisory Board and State committee members will be in attendance on Friday, April 18 as faculty and student researchers present their research and discuss ways to enhance collaboration among the four research institutions.

Olsen will discuss the future direction expected of the program and the Foundation itself.

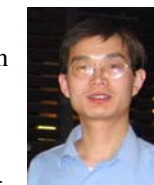
Dr. Denise Barnes, NSF EPSCoR program director, will speak about changes pertaining to EPSCoR and the upcoming request for proposals.



EPSCoR funds provide new faculty positions

New hiring continues in the Computational Chemistry area at the University of Southern Mississippi (USM) and Jackson State University (JSU). These new faculty members will help carry out research at two of the four Mississippi research institutions. New hires include Yong Zhang at USM and Glake Hill at JSU.

Yong Zhang is an assistant professor in the Department of Chemistry and Biochemistry at USM. He received his doctorate at Nanjing University in China in 1997 and completed post doctoral work as a research scientist at the University of Illinois at Urbana-Champaign before joining USM.



Zhang's research interests include Computational Chemistry, Physical and Biophysical Chemistry, and Inorganic and Bioinorganic Chemistry. His current research includes: *High Accuracy Spectroscopic Property Calculations; Biomolecular Structure Refinement and Determination; and Metallobio-Molecules in Cellular Regulation and Signaling and Human Diseases*. More information on each of these can be seen at: <http://www.usm.edu/chem/Research/Zhang.pdf>.

Dr. Robert Bateman, Chair and Professor of Biochemistry in the Department of Biological Sciences at USM said "the USM Department of Chemistry and Biochemistry is pleased to have Dr. Yong Zhang join us as an assistant professor. Dr. Zhang is a biophysical chemist who uses computational techniques to analyze the structures of metal-containing proteins, particularly those involved in human diseases. His work bridges the gap between computational structural biology and the organometallic chemistry pursued by several chemists in the department."



Glake Hill is an assistant professor in the Computational Center for Molecular Structure and Interactions in the Department of Chemistry at JSU. He earned his doctorate degree in Chemistry at Jackson State University in 2003 and was a President's Research Postdoctoral Fellow at the University of California, Berkeley.

Hill's research interests include DNA methylation using ab initio quantum chemistry. The other area that he is involved includes materials science, specifically cluster formation and utilizing DNA fragments to improve nanotube properties.



From the director

Mississippi State University is pleased to host the annual Mississippi EPSCoR State Meeting on Friday, April 18, 2008. Mississippi EPSCoR is a collaborative effort of Mississippi's four research institutions through the Mississippi Research Consortium (MRC). The MRC is composed of the chief research officers representing Jackson State University, Mississippi State University, the University of Mississippi, and the University of Southern Mississippi.

The meeting will begin at 8 a.m. on Friday morning with EPSCoR researchers representing Mississippi's four research institutions discussing current collaborative research efforts among the universities with the National Advisory Board members and the Mississippi EPSCoR State Committee. Following these discussions, each Computational Science research focus group, along with Outreach and Education, will present the results of their current research to all students, faculty, and guests in attendance. Students will showcase their research in poster sessions in the early afternoon.

The day will conclude with the National and State Advisory members providing feedback to the EPSCoR researchers concerning ways that they can continue to enhance collaboration in research and in education and outreach among the four research institutions. In preparation for the submission of a proposal to seek new funding from EPSCoR, the boards will provide input to the EPSCoR team about building on the current research to further build human capacity in key areas and our competitiveness and reputation in the national arena.

We are excited to have Dr. Kathie Olsen, Deputy Director of NSF and Dr. Denise Barnes, NSF EPSCoR Program Director, join us for our state meeting and look forward to showcasing the outstanding research being conducted by our scientists and students. We are utilizing education and outreach to increase diversity in the computational sciences.

Sandra N. Hingle

Students/faculty attend MCBIOS 2008 conference in Oklahoma City

Faculty and students from the Mississippi Research Consortium recently attended the Fifth Annual Conference of the MidSouth Computational Biology and Bioinformatics Society (MCBIOS) in Oklahoma City, Oklahoma. The theme of the two day conference was "Systems Biology – Bridging the Omics."

The conference included technical sessions and panel discussions on sequence analysis, image processing, microarray analysis, protein structure/function prediction, gene finding algorithms, genomics, metagenomics, pathway analysis, systems biology, and metabolic/cellular simulations.

William Sanders, a graduate student from Mississippi State University (MSU) presented a session titled "Mass Spec Identification of Expressed Protein Sequence Tags;" Nan Wang, a graduate student from Mississippi State University presented a session titled "Distance-based Outlier Detection Model for

Improving MS/MS Peptide Identification Confidence," and Dr. Youping Deng, Assistant Professor at the University of Southern Mississippi presented "Machine Learning Recognition of Metabolomic Lipid Markers for Prostate Cancer."

The conference attracted 140 participants with 68 posters being submitted. Student talk winners included Wang of MSU, second place; Sanders of MSU, third place. In the poster session competition, Prashanti Manda from the Department of Computer Science and Engineering (CSE) at MSU received an honorable mention for her poster which was co-authored by Chamali Thanthiriwatte in CSE and Bart van den Berg of the College of Veterinary Medicine at MSU.

Dr. Dawn Wilkins, president-elect MCBIOS and Associate Professor from the University of Mississippi spoke on the upcoming MCBIOS 2009 Conference which will be held at Mississippi State University.

Seed grant recipient presents at SEARCDE

Dr. Seth Oppenheimer was just one of many scientists who attended the 27th Southeastern Atlantic Regional Conference on Differential Equations (SEARCDE) at Murray State University in Kentucky.

Oppenheimer is a recipient of a Mississippi Computational Biology Consortium (MCBC) seed grant. MCBC is a research focus of the Mississippi Computational Sciences Network. MCSN is funded through the National Science Foundation,



Experimental Program to Stimulate Competitive Research (EPSCoR). The seed grant, in the amount of \$25,000, allowed Oppenheimer and research partner Gary Ervin, to further their research efforts at Mississippi State University (MSU). Oppenheimer and Ervin's seed grant research is titled, "Integrating Effects of Land Use Change on Invasive Plant Species Distribution Into An Invasive Plant Atlas for the Mid-South."

Oppenheimer's SEARCDE presentation, "A Model For the Spread of An Invasive Species," spoke to the geographic spread of a wind-dispersed (continued on page 3)

Engineers reach across disciplines to make a difference

A vortex is the swirling of air that you see off the wing tip of a jet. This same type of vortex occurs as air passes through the bronchial tubes of your lungs. That explains why Dr. David Thompson, Associate Professor of Aerospace Engineering at Mississippi State University, who is an expert in fluid dynamics, is modeling the air-flow in bronchial tubes. His research funded by the National Science Foundation's EPSCoR project, will help medical experts understand how to design better techniques for aerosol drug delivery.

"What happens is that the aerosol droplets can get caught in a vortex's swirling cycle and the medication is then less effective because it never settles inside the bronchial tube," explained Thompson.

Thompson normally uses his fluid dynamic expertise to simulate the flow of air around jet engines, wings of aircraft, and rocket engines of spacecraft. When the request came to apply that same knowledge to study the human lung, Thompson decided he needed assistance from someone more familiar with the human anatomy. That is when he hired Charla Lindley, a senior bio-medical engineering major.

"I really didn't know what I was get-

ting into when I asked Dr. Thompson if I could have a job. Most bio-medical engineering students are working with cells in a lab," but Lindley expressed that she wanted to apply her bio-medical engineering knowledge in a different way. "Eventually, I want to work with prosthetics, and that requires building the designs and simulating their motion on a computer and then building them for real. Here, I'm using similar computational software on this project."

While the project is helping Lindley develop skills to become a more effective bio-medical engineer, it also is helping her realize the value of having team members who have completely different sets of expertise. Bela Soni, a Ph.D. computational engineering student, is studying how to simulate models of the human body—particularly the lungs.

"When I started this I was solely studying computational engineering," explained Soni. "Its application is normally more in the simulation of turbines or missiles or airplanes and this is a biological application." She also said that working on this project has helped her realize one of her dreams - "it is the main focus of my research and it's very interesting. Actually I always wanted to become a doctor, so at least I can do something that can



Standing is Lindley; seated is Soni

help doctors," she concluded.

The next steps involve Thompson and his two students sharing their computational fluid dynamic results with medical center experts. The payoffs of the research are that Lindley will have a credit as a co-author of a journal, an accomplishment that very few undergraduates can claim, and future diabetes patients may potentially have non-evasive ways of taking insulin.

"The thing that I think is really neat about this is Charla Lindley knows more about biology than the two of us put together," said Thompson. He ended with, "I have a lot of experience in the simulation side, but Bela Soni really is the one who knows how to simulate air flows in the lungs, so it is a great example of how team members with different academic backgrounds can collaborate and make a difference."

SEARCDE presentation (continued from page 2)

invasive shrub, as influenced by human disturbances that provide open-canopied low competition habitat. Oppenheimer explains that they (he and Ervin) have "developed a preliminary hybrid lattice model operating in two stages. The model divides the domain into spatial nodes, each of which has a carrying capacity and intrinsic growth rate for a continuous logistic growth model for plant population. There is then a seed dispersal stage with each lattice node having a probability of plant establishment depending on seed load. The old popula-

tion is taken as the initial condition in previously occupied nodes and the established seedling population is taken as the initial condition in formally unoccupied node and the logistic stage is run again."

Oppenheimer, a professor in the Department of Mathematics and Statistics and Computational Engineering, received his doctorate in mathematics from the University of Texas at Austin. His research interests are partial differential equations, applied functional analysis, ordinary differential equations, and mathematical modeling.

Ervin is an associate professor in the Department of Biological Sciences at MSU. His research program has two general areas of focus: ecology of invasive species and wetland plant ecology. His work involves projects ranging from plot-scale studies of mechanisms enabling plant colonization and persistence to regional distribution of invasive plants and plants that host invasive insect herbivores.

Financial support for the conference was provided by the National Science Foundation and Murray State's College of Science, Engineering and Technology and Office of Academic Affairs.