

# Innovations through Computational Sciences

NSF-EPS 0556308 (2006-2009)

## **Mississippi EPSCoR**

**Jackson State University, Mississippi State  
University, the University of Mississippi,  
the University of Southern Mississippi**

# Mississippi EPSCoR

- Joint project of the Mississippi Research Consortium (MRC)
  - Jackson State University (JSU)
  - Mississippi State University (MSU)
  - University of Mississippi (UM)
  - University of Southern Mississippi (USM)
- P.I. : Dr. Sandra H. Harpole, Associate Vice President for Research, MSU

# Mississippi EPSCoR

- First funded in 1989
- Goal to build research infrastructure
- Significant increases in
  - Proposal submissions (1,327 to a total of 31,954)
  - Awards (799 to a total of 28,207)
  - Publications
  - Collaborations

# Innovations through Computational Sciences

- **Goal:**
  - **To establish a national prominence in the computational sciences by enhancing research capacity in the theme area of computational sciences building on the existing strengths in high performance computing**

# Innovations through Computational Sciences

- **Theme Areas**
  - **Computational Biology** – JSU, MSU, USM
  - **Computational Chemistry** – JSU, UM, USM
  - **Multi-Scale Biosystem Simulation and Modeling** – JSU, MSU, UMMC
- **Education and Outreach**
- **Evaluation**

# Innovations through Computational Sciences

- **Specific Goals:**
  - **Building a national prominence in the theme area of computational sciences**
  - **Increasing research capacity resulting in national competitiveness**
    - **Recruitment of outstanding new faculty with competitive "start-up packages"**

# Innovations through Computational Sciences

## **Specific Goals:**

- **Increasing research capacity resulting in national competitiveness**
  - **Support and mentoring of new and existing faculty in interdisciplinary computational sciences research**
  - **Recruitment of excellent graduate students**
  - **Enhancement of computational science infrastructure**

# Innovations through Computational Sciences

- **Specific Goals:**
  - **Expanding collaboration among MRC institutions and with outside laboratories**
  - **Growing the pipeline in science, technology, engineering and mathematics (STEM) by**
    - **Expanding opportunities for women and underrepresented groups in the computational sciences**
    - **Increasing the number of graduate students**
    - **Interfacing with K-12 teachers and students.**

# Innovations through Computational Sciences

- **Specific Goals:**
  - **Fostering the economic development of the state and nation through development of intellectual property in the computational science area and its commercialization to new spin-off or to partner companies.**

# *Computational Biology*

- Increase number of faculty and staff with expertise in both computational and biological disciplines
  - Recruit five new computational biology faculty
  - Establish graduate research fellowships and seed grants in computational biology
  - Facilitate statewide methods of communication, collaboration and distance learning

# *Computational Biology*

- Scientific focus
  - New techniques in computational biology
  - New paradigms in high performance computing
  - Biological ontology

# *Computational Biology*

- Dr. Susan Bridges-Professor, Computer Science and Engineering (MSU)
- Dr. Shane Burgess-Associate Professor, CVM Basic Science (MSU)
- Dr. Hari H. P. Cohly-(JSU)
- Dr. Raphael D. Isokpehi-(JSU)
- Dr. Frank Moore (USM)

# *Computational Chemistry*

- Cross-disciplinary research to meld computational sciences with experimental data
  - Solvation and Ligand-Biomolecule Interactions
  - Computational Chemistry for Environmental and Industrial Applications
  - Material Chemistry – Metal Complexes, Novel Clusters and Nanoparticles

# *Computational Chemistry*

- Dr. Robert Bateman-Chair & Professor, Chemistry & BioChemistry, (USM)
- Dr. Steven Davis-Professor of Chemistry and Biochemistry, (UM)
- Dr. Glake Hill (JSU)
- Dr. Jerzy Leszczynski (JSU)

# Multi-Scale Biosystem Simulation and Modeling

- Biosystem simulation – technique of describing mathematical approximations & computing solutions to approximations using numerical techniques
  - Refinement of the integrative model of human physiology (UMMC, MSU)
  - Multi-scale simulations of an artificial liver device (MSU, UMMC)

# Multi-Scale Biosystem Simulation and Modeling

- Biosystem simulation
  - Fluid dynamics of lung respiration and meso-scale aerosol deposition (MSU, JSU, UMMC)

# Multi-Scale Biosystem Simulation and Modeling

- Dr. Shahrouz Aliabadi-(JSU)
- Dr. Greg Burgreen, Associate Research Professor, Computational Simulation & Design, MSU
- Dr. Robert Hester, Professor Physiology and Biophysics, UM Medical Center
- Dr. David Marcum, Director, SIM Center, MSU

# *Education and Outreach*

- Common themes
  - Introduce students to inquiry and team-based interdisciplinary research
  - Inform students about careers in computational science
  - Provide students with the support, encouragement and tools needed to continue in related discipline

# *Education and Outreach*

- Educational product development
  - Curricular paths
  - Interdisciplinary courses
  - Computational biology/chemistry/modeling modules

# *Education and Outreach*

- High school juniors/seniors
  - Computational science laboratory experience
  - Mississippi EPSCoR scholarship
- High school teachers/counselors
  - Research and career awareness workshop

# *Education and Outreach*

- Undergraduate students
  - High school recruitment
  - Academic preparation and involvement in a learning community
  - Undergraduate research
  - Statewide networking symposium for undergraduate researchers and mentors

# *Education and Outreach*

- Pamala Heard (JSU)
- Dr. Sherry Herron, Assistant Professor/Director of Science and Math Education, USM
- Dr. Peter Sukanek-Chair and Professor of Chemical Engineering, UM
- Dr. Giselle Thibaudeau-Associate Professor/Director Electron Microscopy, MSU

# *Evaluation and Assessment*

- Evaluation team from JSU, MSU, UM and USM
  - Ms. Georgia Hackney, Research Associate I, Center for Science, Mathematics & Technology, MSU
  - Dr. Sherry Herron, Assistant Professor/Director of Science and Math Education, USM
  - Dr. Amy Wells, Associate Professor of Leadership and Counselor Education, UM
  - Dr. Gregory Opara-Nadi, Program Evaluation Specialist, JSU