

#### **Mission**

To foster interdisciplinary research in both the fundamental understanding of and application of all the natural sciences.

In particular, to model and develop integrated computational environments and crosscutting tools that allow a comprehensive, cross-disciplinary approach to problem-solving.

# NSF Engineering Research Center (ERC) for Computational Field Simulation, 1990-2001

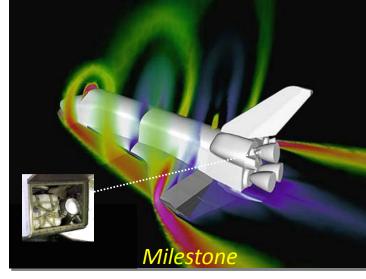
**Mission:** To reduce the time and cost of complex field simulations for engineering analysis and design.

## Cross-Disciplinary Research Team with a Common Focused Mission

Science & Engineering Faculty; ASE, CE, CS, ECE, MA, ME, PH

#### Mission Related Educational Programs

Computational Engineering MS & PhD Program Related CME, ASE, CS, ECE, MA, ME courses Undergraduate Outreach Programs



During the 1998 STS-95 (John Glenn) Mission the drag chute door fell off at launch. A shuttle simulation, completed by the ERC allowed the ERC to reduce the solution time from 2 months to 2 days.



High Performance Computing Collaboratory

and service.

## Definitions and Goals of the High Performance Computing Collaboratory

## The High Performance Computing Collaboratory (HPC<sup>2</sup>) is a coalition of member centers and groups that share

<b>∟</b> a	common core objective of advancing the state-of-the-art in computational science and engineering using high performance computing,
□a	common approach to research that embraces a multi-disciplinary, team-oriented concept,
□aı	nd a commitment to a full partnership between education, research,

HPC<sup>2</sup> aims to become the nation's premier interdisciplinary highperformance computing research facility.

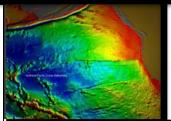


## The Centers/Institutes of the High Performance Computing Collaboratory

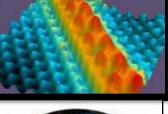
**CAVS** is an interdisciplinary center providing engineering, research, development, and technology transfer teams focused on complex problems, such as those encountered in technologies designed to improve human mobility. Development efforts provide short-term solutions relevant to regional manufacturers while the core research builds longer-term knowledge needed for sustained economic development. Students gain valuable project experience that compliments their formal classroom learning.

Center for Advanced
Vehicular
Systems (CAVS)









## Geosystems Research Institute (GRI)

**GRI aims to** be a world leader in advancing the state-of-the-art in spatial technologies and resource management. **The Institute's mission is** to understand Earth's natural and managed systems and provide comprehensive solutions for socioeconomic and environmental requirements, leading to an improved quality of life.



## Northern Gulf Institute (NGI)

**NGI aims to** be a regional leader providing integrative research and education to improve the resiliency and conservation of the Northern Gulf of Mexico. **NGI** conducts high-impact research and education programs focused on integration of the land-coast-ocean-atmosphere continuum; integration of research to operations; and integration of individual organizational strengths into a holistic program. NGI will contribute to the recovery and future health, safety, resilience and productivity of the region, through sustained research and applications in a geospatial and ecosystem context.



## Research Expenditures, Funding, Personnel of the High Performance Computing Collaboratory

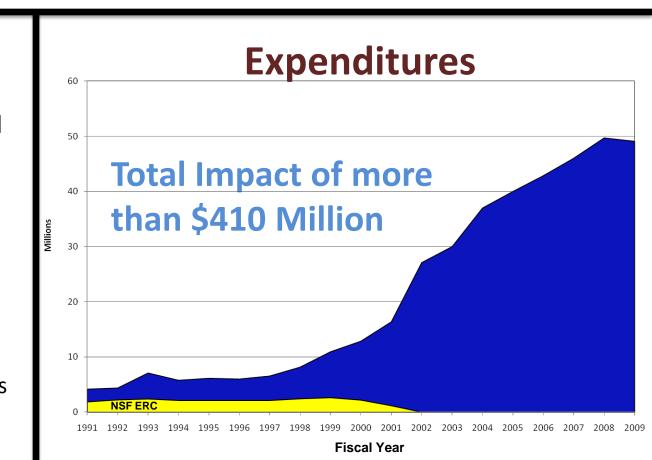
## **Major External Funding Agencies**

DoD, NASA, NOAA, USDA, NSF, DIA, DoE, USGS, USDOT, NIEHS, NIST, HUD, DoL, EPA, SBA, MS-DEQ, MS Space Commerce Initiative, MDA, Bell Helicopter, Boeing, Northrop Grumman, Sentel Corp., Miltec Corp., General Motors, ESI Group

#### **Personnel**

486 Total HPC<sup>2</sup> Personnel

70 Academic Faculty
38 Research Faculty
16 Postdoctoral
91 Research Associates
27 Staff
134 Graduate Students
110 Undergraduate Students





## Academic Affiliations of the High Performance Computing Collaboratory

#### **College of Agricultural and Life Sciences**

Ag Econ, BioChem and Molecular Biology, Entomology and Plant Pathology, Plant & Soil Sciences

#### **College of Arts & Sciences**

Biological Sciences, Chemistry, Geosciences, Math and Statistics, Physics and Astronomy, Sociology Anthropology and Social Work, Psychology

#### **College of Veterinary Medicine**

#### **College of Engineering**

Aerospace, Ag & Bio, Civil, Chemical, Computer Science, Electrical & Computer, Industrial, Mechanical

#### College of Architecture, Art, & Design

**Art** 

#### **College of Business and Industry**

**Finance and Economics** 

#### **College of Forest Resources**

Forestry, Wildlife and Fisheries

#### **Educational Program**

M.S., more than 75 grads

Ph.D., more than 25 grads

#### **Computational Mathematics**

(numerical analysis, numerical solutions to PDEs, numerical linear algebra)

#### **High-Performance Computing**

(parallel algorithms, software engineering, computer architecture)

## Application area from engineering or physical science

(computational fluid dynamics, electromagnetics, structural analysis, hydrodynamics, geospatial modeling)



#### **High-Performance Computing Systems**

Talon: 3072 processors,

6 TB RAM

Raptor: 2048 processors,

4 TB RAM

Matador: 512 processors,

**512 GB RAM** 

Maverick: 384 processors,

**480 GB RAM** 

## **Infrastructure and General Purpose Computing Systems**

145 servers

#### **Storage**

250 TB of high-speed disk storage

2 PB of near-line storage

#### **Desktops/Laptops**

325+ Faculty/Staff desktops and

laptops

250+ Student desktops

#### **Networking**

5300+ data ports



- IBM iDataPlex
- 3072, 2.8-GHz6-way Westmere
- 6 TB of RAM
- Quad-data rate
  Infiniband





Mississippi State University is now home to one of the world's greenest supercomputers, according to the Green500 List released this month (June 2010).

Ranked as the most energy efficient general-purpose supercomputer in the world

7<sup>th</sup> most energy efficient system overall

Can perform nearly 420 million calculations for every watt of electricity it uses

18<sup>th</sup> fastest computer in any university in the United States

331st most powerful computer in the world

Mississippi State has been on 18 of the past 29 Top500 Lists dating back to June 1996.



### **Facilities**

#### **HPC Building – Starkville**

• 71,000 square feet

#### **CAVS Building – Starkville**

• 57,000 square feet

## NASA Stennis Space Center – MS Gulf Coast

- 2 large suites in Bldg. 1103
- Construction of ~40,000 sq.ft.
   facility to begin in June 2010









## <u>Virtual Environment for</u> <u>RealTime EXploration</u>

Fakespace FLEX<sup>TM</sup> Virtual Reality Device

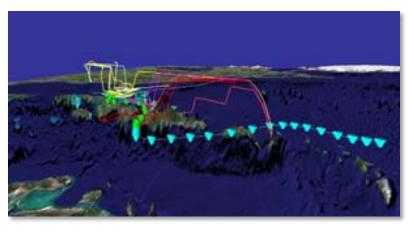
Three projected walls plus floor

Acoustic motion tracking

Active and passive 3-D stereo viewing

Reconfigurable into a Powerwall for large displays







### **Publishing**

- Brochures
- Annual Reports
- Posters
- Flyers/Handouts
- Business Cards/Stationary
- Web Design
- Photography
- Exhibits/Displays
- Logo Creation
- Video/Audio Production
- Copywriting/Editing





## **Center for Computational Sciences**

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#### **Mathematics**

Ratnasingham Shivaji , Director, W.L. Giles Distinguished Professor

Hyeona Lim, Associate Professor Seth Oppenheimer, Professor Shantia Yarahmadian, Assistant Professor

Xingzhou Yang, Assistant Professor

#### **Physics**

Seong-Gon Kim, Associate
Director, Associate Professor
Anatoli Afanasjev, Professor
Deepankgar Dutta, Assistant
Professor

Gautam Rupak, Assistant Professor Mark Novotny, Professor and

Dept. Head

Matthew J. Berg, Assistant Professor

Torsten Clay, Associate Professor

## **Electrical & Computer Engineering**

Sherif Abdelwahed, Assistant Professor

#### **Biological Sciences**

Christopher Brooks, Assistant Professor

Diana C. Outlaw, Assistant Professor

Lisa Wallace, Assistant Professor Mark Welch, Assistant Professor Vincent Klink, Assistant Professor

#### **Chemistry**

Edwin A. Lewis, Professor and Dept. Head Steven Gwaltney, Associate Professor

#### **Computer Science**

Changhe Yuan, Assistant Professor Ioana Banicescu, Professor Song Zhang, Assistant Professor

#### **Statistics**

Professor

Meng Zhao, Assistant Professor

QiQi Lu, Associate Professor

#### **Industrial Engineering**

Mingzhou Jin, Associate Professor

#### College of Veterinary Medicine, Basic Sciences

Henry X.-F. Wan, Assistant Professor

#### Affiliated faculty

Jagadish P. Singh, Research Professor, Institute of Clean Energy and Technology.

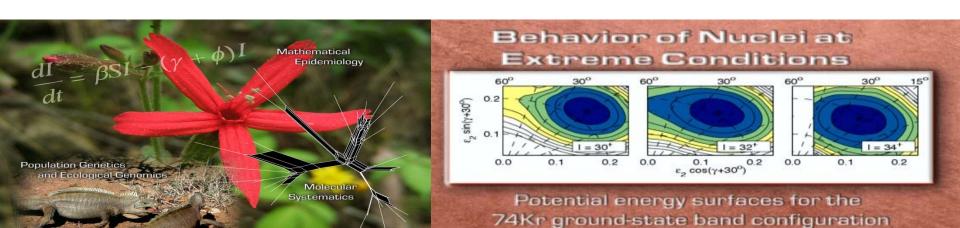
Yang Ki Hong, Professor &
E.A.Larry Drummond
Endowed Chair of Computer
Engineering, Dept. of
Electrical & Computer
Engineering, University of
Alabama, Tuscaloosa.



## **Center for Computational Sciences**

## Some Research Foci

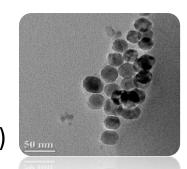
- Computational Ecology and Evolutionary Biology
  - Computational Physics
  - Computational and Applied Mathematics
    - Computational Statistics
  - Modeling Visualization and Optimization





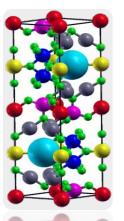
## FY 2011 Federal Initiative Proposal (request: \$7 Million /3 years): Advanced Materials Design for Nano Devices

Mississippi State University proposes to conduct transformative research to develop unique and innovative materials and magnetic memory elements for high-density nanoscale memory devices and nanosensors for chemical warfare agents in support of the Nano Electronics Team of Sensor and Electron Devices Directorate (SEDD) at the U.S. Army Research Laboratory (ARL).



#### P.I. Seong-Gon Kim (MSU, Physics)

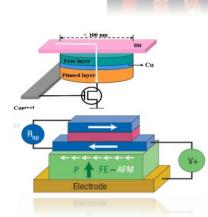
Administrator: R. Shivaji (MSU, CCS Director, Mathematics)



Interdisciplinary team: Computational Physics, Experimental Physics, Chemistry, Mathematics, Electrical and Computer Engineering, Materials Science

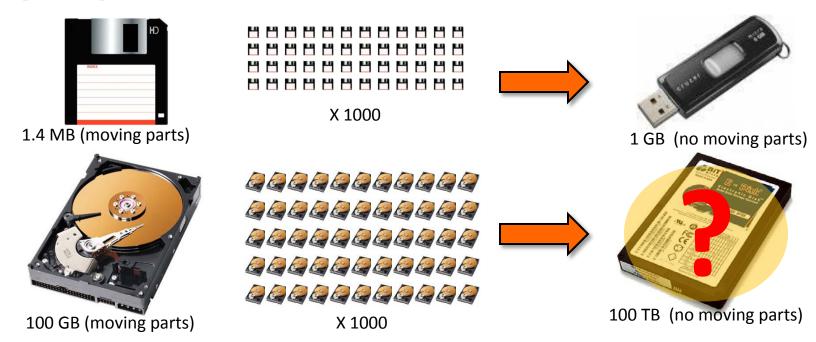
**Education:** 14 doctoral students and 7 postdocs will be involved in research each year

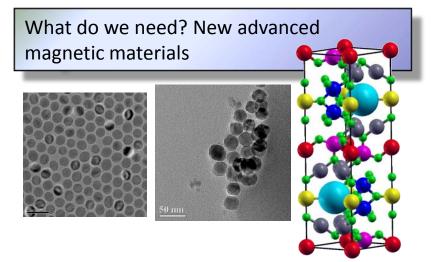




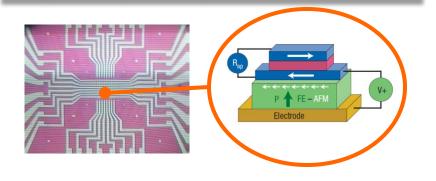


### **Overview**





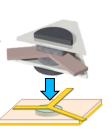
What will we have? Actual prototypes of high-density memory cells





## **Economic Impact**

- ☐ Will bring products to the market to be used for both civilian and national security applications.
- Will bring research and manufacturing work for next generation of high-tech equipments/devices critical to national security to the State of Mississippi.
  - Miniature GHz circulators and radars
  - Insect-sized micro air vehicles (MAV)
  - Lightweight communication systems
  - Biological and chemical sensor devices
- New ultra-high-density memory devices developed in the proposal will create a multi-billion dollar market for the information storage industry and increase information security significantly.
- ☐ The success of this project has a strong potential to bring new high-tech manufacturing work to the State of Mississippi. Support letters:
  - Seagate Technology, Fremont, CA;
  - Western Digital, San Jose, CA;
  - Custom Sensors & Technology, Frenton, MO.

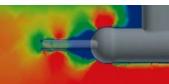


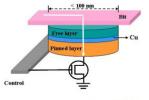


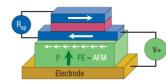




















## **Federal Agency Collaboration**

**Federal Agency: Department of the Army** 

Program Officer: Dr. Madan Dubey

Nano Electronics Team Leader Army Research Laboratory

#### **Sensor and Electron Devices Directorate**

**Title: University and Industry Research Centers** 

Army PE/Project: 61104.J13 OSD

PE #: 0601104A

## **Support Letter**



DEPARTMENT OF THE ARMY

UNITED STATES ARMY RESEARCH LABORATORY 2800 POWDER MILL ROAD ADELPHI, MARYLAND 20783-1197

REPLY TO THE ATTENTION OF

September 10, 2008

10:
Dr. Ratnasingham Shivaji, Director
Center for Computational Sciences (CCS)
Box 9627, Mississippi State University
Mississippi State, MS 39762.
Tel: (662) 325-4036, E-mail: shivaji@ra.msstate.edu

FROM: Dr. Madan Dubey Nano Electronics Team Leader SEDD; AMSRL-SE-RL 2800 Powder Mill Road Adelphi, MD 20783-1197

Ref: Army Research Lab interest in the "Advanced Materials Design for Nano Devices" proposal from the Center for Computational Sciences (CCS) at Mississippi State University (MSU)".

Dear Dr. Shivaji:

First, please accept my highest appreciation and profound thanks for your visit with your colleagues Prof. Kim and Prof. Singh to the Army Research Lab, Adelphi, MD on May 15, 2008 for an exciting seminar and very stimulating discussion on future MSU-ARL collaboration. We are very impressed with the proposed research on "Advanced Materials Design for Nano Devices" at the Center for Computational Sciences (CC)3 at Mississippi State University. Your visit to ARL and the multiple conference call discussions were very helpful to learn about your proposal. In fact, we are very interested in all the tasks listed in this proposal, namely, "Task 1: Optimizing Magnetic Properties of Hexaferrites", "Task 2: Current-Rewritable Nanoscale Magnetic Memory Cells", "Task 3: Voltage-Rewritable Multiferroic Memory Cells" and "Task 4: Nanosensors for Chemical Warfare Agents." I must add that we are also very impressed with

for an exciting seminar and very stimulating discussion on future MSU-ARL collaboration. We are very impressed with the proposed research on "Advanced Materials Design for Nano Devices" at the Center for Computational Sciences (CCS) at Mississippi State University.

explosives and chemical and biological agents. Thus, these projects will lead to dual use of the technologies developed. The collaboration of ARL and CCS/MSU will quickly bring products to

Devices" at the Center for Computational Sciences (CCS) at Mississippi State University. Your visit to ARL and the multiple conference call discussions were very helpful to learn about your proposal. In fact, we are very interested in all the tasks listed in this proposal, namely, "Task 1: Optimizing Magnetic Properties of Hexaferrites", "Task 2: Current Pewritable Nanescale

May, 2008 – Kim, Singh, and Shivaji \$15,000 seed funding (2010)



## **Support from Industries**



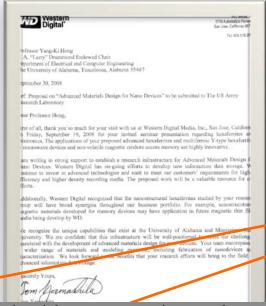
Vice Pres. of Seagate Technology

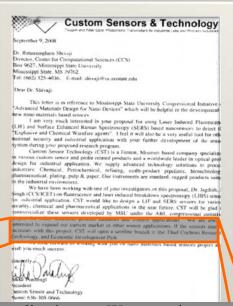


Vice Pres. of Western Digital Inc.









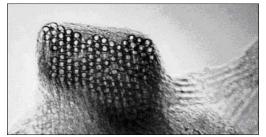
project for other industrial process monitors and control applications. We are always interested to around our current market in other sensor applications. If the sensors market increases with this project, CST will open a satellite branch in the Thad Cochran Research, Technology, and Economic Development Park

we rook forward to working with you on nano materials based sensors project and

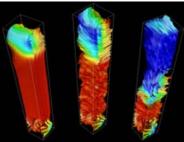


## **Expanding MSU Capabilities**

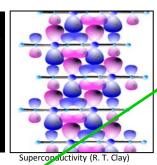
Research in materials science is one of the leading thrust areas of research at the CCS – Superconductivity, nanostructures, micromagnetic simulations.

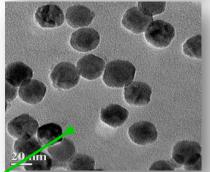


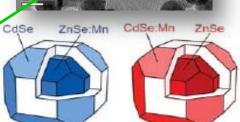
Science 273, 483 (1996) – Crystalline ropes of carbon nanotubes (S. Kim with Nobel laureate R. Smalley)



Micromagnetc simulation (M. Novotny)







Erwin, et al., "Doping Semiconductor Nanocrystals," Nature 436, 91 (2005)

The project provides MSU team an opportunity to expand its expertise to advanced magnetic materials.

Prof. Hong of UA is one of the highly recognized experts in magnetic nanoparticle synthesis and microcircuit fabrication.

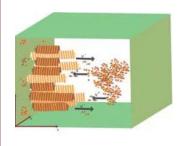
- Inventor of "Pac-man" -shaped Ni<sub>80</sub>Fe<sub>20</sub> thin film elements
- •Recently synthesized world's smallest (< 20 nm) spherical Ba-hexaferrite nanoparticles.
- Dr. S. Erwin of NRL (Task 1 & 3) is one of the world's best experts in nanocrystal doping and theory of magnetism.

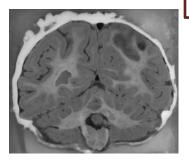


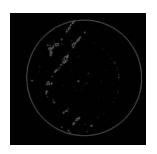
# Recent National Science Foundation (NSF) Proposal (> \$2 million) for a Research Training Group (RTG) Program at Mississippi State University

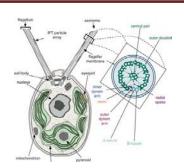


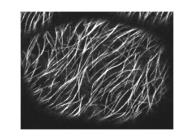
Goal: To promote a research training environment in Partial Differential Equations with Applications in Biology and Materials Science at Mississippi State University by providing a variety of research and teaching activities designed to promote the professional development and education of trainees.

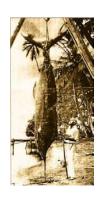












The RTG program will generate a better educated and trained workforce by supporting and training 2 postdoctoral associates, 14 graduate students and 10 undergraduates for strong skills in computers, modeling and applications of the scientific method.

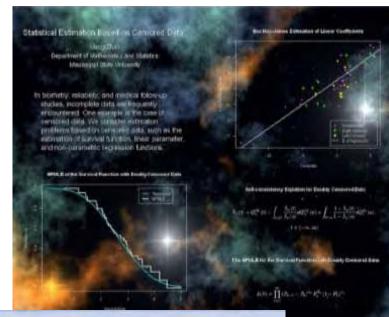


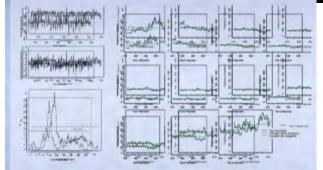
Biologists, Computer Scientists, and Statisticians join to submit an NSF-UBM (National Science Foundation Interdisciplinary Training for Undergraduates in Biological and Mathematical sciences)

proposal

Dr. Christopher Brooks led a team of members, Haimeng Zhang, Lisa Wallace, Huiping Xu and Changhe Yuan in the submission of UBM Group proposal "The Landscape Genetics of Plant-Pollinator Interactions-Integrating Models and Data". This project aims at three year research experiences for MSU undergraduate participants.

Participants will receive a comprehensive educational exposure to mathematical biology while becoming involved in research projects that address important questions in landscape genetics. This initiative is expected to greatly enhance interaction between biologists and mathematicians at MSU.

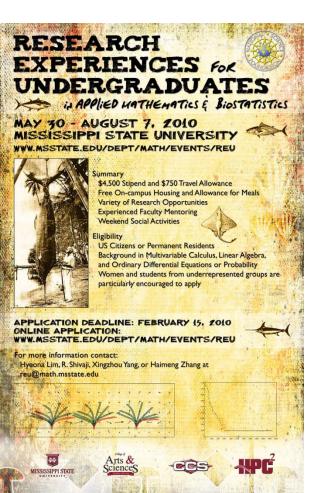






CCS received National Science Foundation funding to host a site for Research Experiences for Undergraduates (REU) program in Applied Mathematics and Biostatistics.





Dr. Hyeona Lim is the Principal Investigator of this project. Dr. Ratnasingham Shivaji is the Co-Principal Investigator and both Dr. Xingzhou Yang and Dr. Haimeng Zhang serve as senior personnel. This REU site project during the summers of 2010 and 2011 is aimed at involving undergraduate students each year in active research under the supervision of these four applied mathematicians and statisticians who are dedicated researchers and mentors. The major area of concentration will be applied mathematics and biostatistics. The cross-cutting themes of the project are image processing, population dynamics, computational mathematical biology, and highly stratified models in biostatistics.

71 applications were received for the 2010 REU program and 7 students were selected among a pool of very strong applicants.

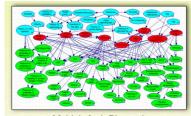
- John Corring, University of Southern Mississippi
- Helen Duke, Providence College
- Justin Hansen, University of Vermont
- ■Emily Poole, University of Arkansas
- Bonnie Roberson,Mississippi State University
- Britanny Stephenson,Mississippi State University
- ■Yicong Yong, University of Florida



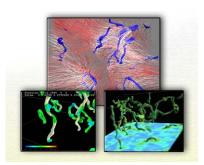
Model-based Self-managing Systems

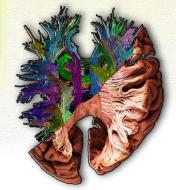
## **Computer Scientists and Engineers join to** submit NSF proposal for research on **Autonomic Computing**

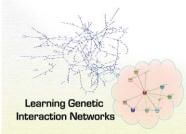
Dr. Ioana Banicescu (PI) and Dr. Sherif Abdelwahed (Co-PI) plan to initiate research on Autonomic Computing at CCS. They have received an NSF planning grant and have submitted a full proposal to NSF and also submitted a proposal for Federal **Initiative funding.** 

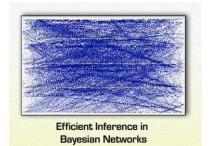


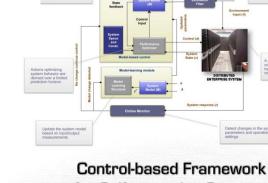
Multiple-fault Diagnosis Using Bayesian Networks











for Self-managing Systems



# NSF Math Institute Proposal White Paper



DEPARTMENT OF MATHEMATICS AND STATISTICS

December 5th, 2008

Dr. Kirk Schulz,

Vice President, Office of Research and Economic Development

Dr. Sandra Harpole,

Associate Vice President, Office of Research and Economic Development

White Paper: Mathematical Sciences Research Institute Proposal

In response to your request to explore possibilities of submitting a Mathematical Science Research Institute Proposal in the near future, our group has developed the following recommendations:

A proposal in one of two general directions is definitely worth pursuit:

[A] An Institute for Discovery and Innovation in the Mathematical Sciences through Computation and Advanced Visualization

[B] An Institute for Mathematics of Materials and Its Applications.

Institute [A] would benefit MSU research in several disciplines, facilitating development of cutting edge multi-disciplinary research in physical systems, biological systems, and geo-systems, which involve applied and computational mathematics, advanced visualizations, and setistics in a significant way.

Institute [B] would considerably strengthen MSU's on-going research efforts in Materia's Science. In particular, such an Institute would help MSU achieve expertise in the area of "Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security", a field recently promoted by the Governing Board of the National Research Council.



A proposal in one of two general directions is definitely worth pursuit:

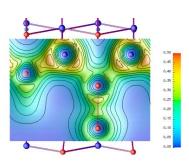
- A) An Institute for Discovery and Innovation in the Mathematical Sciences through Computation and Advanced Visualization
- B) An Institute for Mathematics of Materials and Its Applications

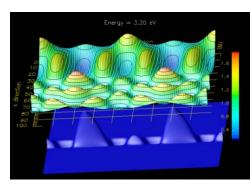
## Material Research Science and Engineering Center (MRSEC) Proposal

- •Center for Multiscale Studies of Engineered Nanocomposites
- •Purpose of the proposal is to develop accurate computational tools to predict material properties without actually manufacturing the new material.



- DOE proposal.
- Project involves development of new nanoscale materials for Hydrogen production.
- Understanding of chemical reactions that occur on the catalyst surface during the reformation process.
- Would provide a new source for hydrogen production from low cost materials.









## Computational Science Training for Undergraduates in the Mathematical Sciences (CSUMS) Proposal

**CSUMS: Undergraduate Research and Training in Differential Equations and their Applications** 

Project is aimed at involving 10 undergraduate students each year in active research under the supervision of applied mathematicians and engineers.

# Focused Research Groups in the Mathematical Sciences (FRG) Proposal

FRG: Numerical Modeling and Industrial Applications in

**Powder Injection Molding for Nanoscale Powders** 

Develop robust and reliable numerical design tools for Particle Injection Molding with nanoscale powders





Heterogeneity

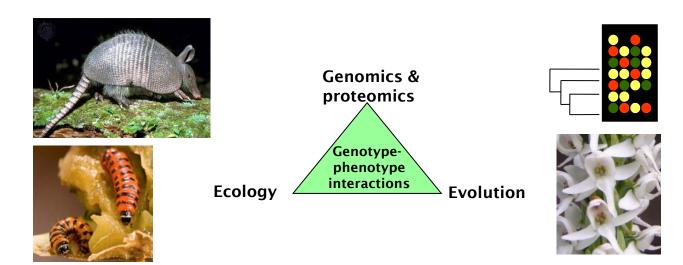
Short filling

### **Major Research Instrumentation Proposal**

NSF Proposal, Jointly with Life Sciences & Biotechnology Institute (LSBI), Institute of Digital Biology (IDB), CCS)

Requests 4 instruments integrated into a single system to support research and education activities in "system biology" at MSU:

- 1. Illumina DNA Analyzer
- 2. LTQ XL electrospray ionization (ESI) linear ion trap mass spectrometry
- 3. LTQ Orbitrap XL ESI mass spectrometry system
- 4. IBM System P computer





### **EPSCoR** Research for Infrastructural Improvement Proposals

Title: MultiScale Atomistics Modeling of Biomolecules and Polymers

The three challenges of the research are:

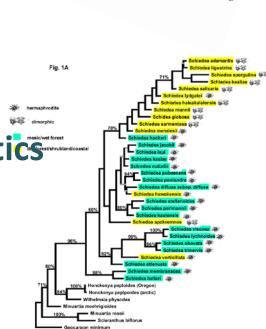
- 1. predicting protein structure and dynamics
- 2. simulating synthetic polymers and their engineering properties
- 3. understanding the interfaces between polymers and nanoparticles

**Title:** Mississippi Consortium for

Evolutionary Ecology CyberInformatics



The research focus area is to develop internet-based infrastructure to guide and facilitate informatics- based evolutionary ecology research.



#### **EPSCoR** Research for Infrastructural Improvement Proposals

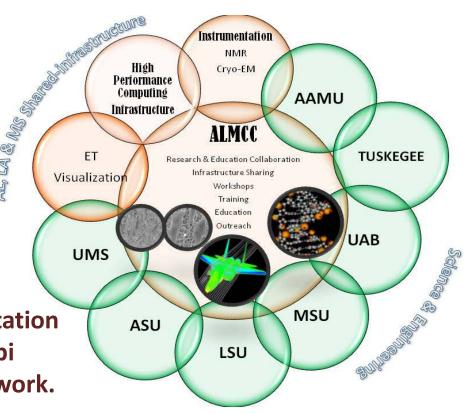
Title: NSF EPSCoR Track II

**White Paper** 

**Key components:** 

**Upgrading Computational Cyber Infrastructure** 

Network and incorporate current scientific and engineering instrumentation in Alabama, Louisiana, and Mississippi onto an advanced tri-state cyber network.





### **Computational Biology Group Meetings**

Several research presentations through out the year

### **CAVS/CCS Joint Forum on Materials Science**

Lectures by mathematicians, physicists, and engineers

### **DARPA – DOD Research Project Meetings**

Nano materials modeling – thermal behavior of nanoparticle solutions subjected to RF excitation

Meetings with Dr. Gary Butler, Director of Tech Outreach, Office of Research

# Joint Research with Institute for Clean Energy Technology (ICET)

Meetings with ICET and CCS members to discuss joint projects.



### Scientific Computing Research Focus Group at MSU

Dr. Ioana Banicescu – Organizer Several meetings throughout the year



## **Computational Biology** Workshop hosted by CCS at MSU

### Mini Workshop on **Mathematical Biology & Computational Modeling**



organized by the Center for Computational Sciences and the Department of Mathematics and Statistics

Friday . March 26 . 2010 HPC2 Rm 20 **Invited Speaker:** Abbas Shirinifard

The Biocomplexity Institute - Indiana University

10:00-11:00 am Multi-Cell Simulation of Development and Disease Using CompuCell3D Simulation Environment

Abbas Shirini Fard - Indiana Biocomplexity Institute

11:15-12:15 pm Mathematical Modeling of Dynamics of Microtubes

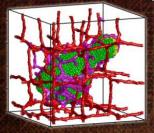
Shantia Yarahmadian - Mississippi State University

1:45-2:45 pm Multi-Cell Simulation of Angiogenesis and Applications

Abbas Shirini Fard - Indiana Biocomplexity Institute

3:00-4:00 pm How Does the Single-Celled Alga Chlamydomonas Swim by its Biflagella? A Mathematical and Mechanical Study

- Xingzhou Yang, Mississippi State Univeristy





Registration is free but limited to 40 participants. For registration and other information, contact Dr. Shantia Yarahmadian (syarahmadian@math.msstate.edu). Please provide your name, e-mail address and your affiliation in your request no later than noon on Wednesday, March 24, 2010.







### **Ecology Workshop organized by CCS at MSU**

Principal Speakers: Dr. Chris Cosner (University of Miami) and Dr. Junping Shi (The College of William & Mary)



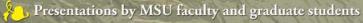
A Workshop Hosted by the Center for Computational Sciences

Mississippi State University August 4-6th 2008, HPC<sup>2</sup> Room 30 For more information contact lisawallace@biology.msstate.edu

#### Speakers:







Dr. Jaffar Ali Shahul-Hameed - Modeling of species invasion

Dr. Chris Brooks - Network models of species invasion

Dr. Gary Ervin - Modeling the spread of invasive plants

Dr. Kevin Knudson - Topological analysis

Dr. Lisa Wallace - Phyloenetic applications in biology

Dr. Mark Welch - Likelihood and Bayesian models in population genetics

Dr. Xingzhou Yang - Biomechanical modeling of cilia and flagella movement

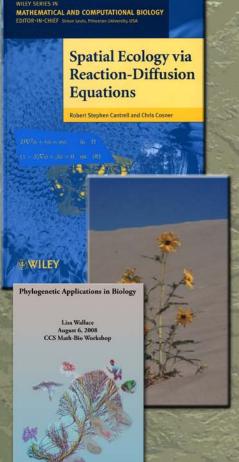
Support from:











# Institute for Mathematics and its Applications (IMA) at University of Minnesota

The Primary Mission of the IMA is to increase the impact of Mathematics by fostering research of a truly interdisciplinary nature, linking mathematics of the highest caliber and important scientific and technological problems from other disciplines and industry.

Mississippi State University is a participating institution of the IMA.

Membership fee: \$10,000 per year.

CCS Coordinates all of MSU's joint activities with the IMA.

#### **Annual Program:**

Mathematics and Chemistry, September 1, 2008, 2008-June 30, 2009
Complex Fluids and Complex Flows September 1, 2009-June 30, 2010
Simulating our complex world: Modelling Computation and Analysis September 1, 2010-June 30, 2011
Mathematics of Information, September 1, 2011–June 30, 2012



Website:

http://www.ima.umn.edu



## **IMA Membership and CCS**

## Participating Corporations

**Boeing** 

**Corning** 

**ExxonMobil** 

**Ford** 

**General Motors** 

Honeywell

**IBM** 

**Lockheed Martin** 

Medtronic

Motorola

**Microsoft** 

Schlumberger

**Siemens** 

**Telcordia** 

### **Participating Institutions**

Air Force Research Laboratory Arizona State University, Tempe Georgia Institute of Technology Indiana University

**Iowa State University** 

**Kent State University** 

**Korea Advanced Institute of Science and** 

**Technology (KAIST)** 

**Lawrence Livermore National Laboratory** 

**Los Alamos National Laboratory (LANL)** 

**Michigan State University** 

**Michigan Technological University** 

#### **Mississippi State University**

Northern Illinois University
Ohio State University
Pennsylvania State University

**Purdue University Rice University Rutgers University** Sandia National Laboratories **Seoul National University Texas A & M University University of Central Florida University of Chicago University of Delaware University of Houston University of Illinois University of Iowa University of Kentucky University of Maryland University of Michigan University of Minnesota University of Notre Dame University of Pennsylvania University of Pittsburgh University of Tennessee University of Wisconsin University of Wyoming Wayne State University Worcester Polytechnic Institute** 

**Portland State University** 



# International Conference Series on Differential Equations and Computational Simulations

The primary objective of these conferences is to provide a joint forum where mathematicians, scientists, and engineers from industries, federal laboratories, and academia exchange research and development ideas.

An overall goal of these conferences is to promote research and education in mathematical and computational analysis of theoretical and applied differential equations.

The unique feature of these conferences is the interaction between mathematicians and engineers.

Researchers from Australia, Belgium, Brazil, Canada, China, Czechoslovakia, France, Germany, India, Indonesia, Japan, Korea, Mexico, Russia, Saudi Arabia, Spain, Thailand, the United Kingdom, and the United States have participated in these conferences.

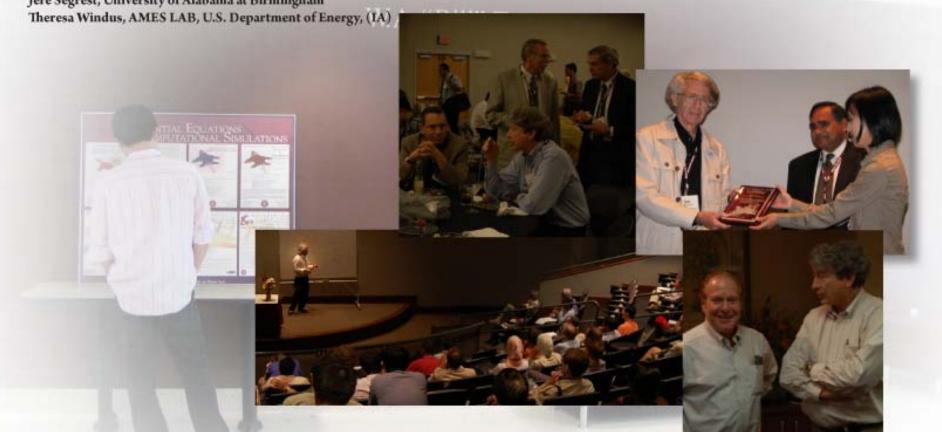
## The Eighth Mississippi State-UAB Conference on Differential Equations and Computational Simulations May 7-9, 2009

The Eighth Mississippi State-UAB Conference on Differential Equations and Computational Simulations was held on May 7-9, 2009, at Mississippi State University, Starkville, Mississippi. There were 13 invited principal lectures presented by:

Douglas Arnold, University of Minnesota
Peter Bates, Michigan State University
Jack Benek, Wright-Patterson Air Force Base, (OH)
Alfonso Castro, Harvey Mudd College, (CA)
Pavel Drabek, University of West Bohemia, Czech Republic
Gisele Goldstein, University of Memphis, (TN)
Philip Maini, University of Oxford, United Kingdom
Scott Morton, Eglin Air Force Base, (FL)
Tinsley Oden, University of Texas at Austin
Stanley Osher, University of California at Los Angeles
Peter Polacik, University of Minnesota
Jere Segrest, University of Alabama at Birmingham

A total of 147 participants and 20 international participants came from 12 different countries. The 2009 DE Conference was dedicated to Joe F. Thompson, W. L. Giles Distinguished Professor of Aerospace Engineering, for his outstanding and continuing contributions to Mississippi State University. 13 principal lectures and 89 contributed talks were delivered. We supported 50 graduate students/new Ph.D's using the NSF grant.

Atlas Conferences, Electronic Journal of Differential Equations (EJDE), Institute of Mathematics and its Applications (IMA) and National Science Foundation (NSF) were the co-sponsors for this conference.



## The Seventh Mississippi State-UAB Conference on Differential Equations and Computational Simulations November 1-3, 2007

The Seventh Mississippi State-UAB Conference on Differential Equations and Computational Simulations will be held on November 1-3, 2007, at Doubletree Hotel, Birmingham, Alabama. There were 12 invited principal lectures presented by:

Oscar Bruno, California Institute of Technology
Chris Cosner, University of Miami
Jeff Crandall, University of Virginia
Norman Dancer, University of Sydney, Australia
Joshua Epstein, The Brookings Institution
Lisa Fauci, Tulane University
YanYan Li, Rutgers University
Jean Mawhin, University of Catholique de Louvain, Belgium
Charles Nietubicz, Army research Laboratory
Jaime Peraire, Massachusetts Institute of Technology
John Rice, IBM TJ Watson Research Center
Peter Takac, University of Rostock, Germany

A total of 95 contributed papers were presented during the threeday conference. The conference was attended by 131 researchers, including those traveling from 7 different countries.

Atlas Conferences, Electronic Journal of Differential Equations (EJDE), Institute of Mathematics and its Applications (IMA) and National Science Foundation (NSF) were the co-sponsors for this conference.







The Sixth Manager State-UAB Conference on Differential Equations and Computational Simulations
tand 13-14, 2005

The Sixth Mississippi State-UAB Conference on Differential Equations and Computational Simulations was held on May 13-14, 2005, at Mississippi State University, Starkville, Mississippi. There were 8 invited principal lectures presented by:

Margaret Cheney, Rensselaer Polytechnic Institute
Lawrence DeLucas, University of Alabama at Birmingham
Thomas Yizhao Hou, California Institute of Technology
Mark Lewis, University of Alberta, Canada
Fang-Hua Lin, Courant Institute of Mathematical Sciences
Robert Meakin, U. S. Army, NASA Ames Research Center
Louis Nirenberg, Courant Institute of Mathematical Sciences
Klaus Schmitt, University of Utah



A total of 90 contributed papers were presented during the twoday conference. The conference was attended by 150 researchers, including those traveling from 9 different countries. This conference was dedicated to Louis Nirenberg in celebration of his 80th birthday, Klaus Schmitt in celebration of his 65th birthday, and their contributions to mathematics. As part of this celebration special sessions were organized. Also a banquet lecture titled "Louis Nirenberg and Klaus Schmitt: The Joy of Differential Equations" was delivered by Jean Mawhin, University of Catholique de Louvain-Belgium. The conference also featured a special lecture by Dr. Mary Ann Horn on the Funding Opportunities in the Mathematical Sciences at the NSF. The post-conference proceedings were published as a special issue of Electronic Journal of Differential Equations (http://ejde.math.txstate.edu/) Conference 15. It contains 25 refereed papers presented at the conference.

Atlas Conferences, Cypress Semiconductors, EJDE, IMA and NSF were the co-sponsors for this conference.

## The Fifth Mississippi State Conference on Differential Equations and Computational Simulations May 18-19, 2001

The Fifth Mississippi State Conference on Differential Equations and Computational Simulations was held on May 18-19, 2001, at Mississippi State University, Starkville, Mississippi. There were 10 invited principal lectures presented by:

Peter Bates, Brigham Young University Carlos Castillo-Chavez, Cornell University Jerome Goldstein, University of Memphis Anthony Ingraffea, Cornell University James Keener, University of Utah David Keyes, Old Dominion University Hiroshi Matano, University of Tokyo, Japan Suresh Menon, Georgia Institute of Technology Wei-Ming Ni, University of Minnesota George Papanicolaou, Stanford University

A total of 69 contributed papers were presented during the twoday conference. The conference was attended by 138 researchers, including those traveling from 7 different countries. The conference also featured a honoring ceremony for Professor Jack Hale, a special lecture by Dr. Henry Warchall on the Funding Opportunities in the Mathematical Sciences at the NSF, and the Banquet Lecture titled "Highway to Space" by Dr. Gary Lyles at NASA Marshall Space Flight Center. The post-conference proceedings were published as a special issue of Electronic Journal of Differential Equations (http://ejde. math.txstate.edu/) Conference 10. It contains 22 refereed papers presented at the conference.

> EJDE, IMA and NSF were the primary co-sponsors for this conference.



# The Fourth Mississippi State Conference on Differential Equations and Companyment Simulations May 21-22, 1999

The Fourth Mississippi State Conference on Differential Equations and Computational Simulations was held on May 21-22, 1999, at Mississippi State University, Starkville, Mississippi. There were 7 invited principal lectures presented by:

Lawrence C. Evans, University of California at Berkeley Charbel Farhat, University of Colorado at Boulder Irene Fonseca, Carnegie Mellon University Ahmed Noor, University of Virginia James Serrin, University of Minnesota Paul Waltman, Emory University Mary Wheeler, University of Texas at Austin A total of 79 contributed papers were presented during the twoday conference. The conference was attended by more than 110 researchers. The post-conference proceedings were published as a special issue of Electronic Journal of Differential Equations (http:// ejde.math.txstate.edu/) Conference 03. It contains 10 refereed papers presented at the conference.

EJDE and NSF were the primary co-sponsors for this conference.



## The Third Mississippi State Conference on Differential Equations and Computational Simulations May 16-17, 1997

The Third Mississippi State Conference on Differential Equations and Computational Simulations was held on May 16-17, 1997, at Mississippi State University, Starkville, Mississippi. There were 9 invited principal lectures presented by:

Walter Allegretto, University of Alberta, Canada Jerry L. Bona, University of Texas Djairo de Figueiredo, University of Campinas, Brazil S.Godunov, Sobolev Institute of Mathematics, Russia Antony Jameson, Princeton University Jean Mawhin, University of Louvain, Belgium Stanley Osher, University of California Klaus Schmitt, University of Utah Joseph Shang, Wright Patterson Air Force Base A total of 75 contributed papers were presented during the twoday conference. The conference was attended by more than 130 researchers, including those traveling from 9 different countries. For those at the Engineering Research Center, it was a very special experience to have had the opportunity to speak with and hear a lecture by Professor Godunov, who is considered as the "grandfather" of computational fluid dynamics research. The post conference proceedings were published as a special issue of the Electronic Journal of Differential Equations (http://ejde.math.txstate.edu/) Conference 01. It contains 18 refereed papers presented at the conference.



EJDE and NSF were the primary co-sponsors for this conference.

## The Second Mississippi State Conference on Differential Equations and Computational Simulations April 7-8, 1995

The second Mississippi State Conference on Differential Equation and Computational Simulations was held on April 7-8, 1995 at Mississippi State University, Starkville, Mississippi. There were 9 invited principal lectures presented by:

Kenneth J. Brown, Heriot-Watt University, Edinburgh, United Kingdom Luis Caffarelli, Institute of Advanced Study, Princeton University David Caughey, Cornell University
Jerome Eisenfeld, University of Texas, Arlington
Jack Hale, Georgia Tech
Peter D. Lax, Courant Institute of Mathematical Sciences
Robert MacCormack, Stanford University
John Mallet-Paret, Brown University
Helen Yee, NASA Ames Research Center

A total of 79 contributed papers were presented during the two-day conference. The conference was attended by approximately 130 researchers, including those traveling from 7 different countries. The post-conference proceedings were published as a special issue of the journal of Applied Mathematics and Computation (89:1-3, 1998). It contains 23 refereed papers presented at the conference.

NSF was a co-sponsor for this conference.

# The First Mississippi State Conference on Differential Equations and Computational Simulations March 19-20, 1993

The first Mississippi State Conference on Differential Equation and Computational Simulations was held on March 19-20, 1993 at Mississippi State University, Starkville, Mississippi. There were 7 invited principal lectures presented by:

Ramesh Agarwall, McDonnell Douglas Research & Development
Alfonso Castro, University of North Texas
Carlos Kenig, University of Chicago
Alan Lazer, University of Miami
Paul Rabinnowitz, University of Wisconsin, Madison
Phillip Roe, University of Michigan
Nigel Weatherill, University College of Swansea, United Kingdom

A total of 68 contributed papers were presented during the twoday conference. The conference was attended by approximately 115 researchers. The post-conference proceedings were published as a special issue of the journal of Applied Mathematics and Computation (65:1-3, 1994). It contains 30 refereed papers presented at the conference.



### Plan for Computational Science Initiative

### Interdisciplinary Graduate Certificate Program (M.S./Ph.D.)

Advanced research and education in Computational Science, including numerical algorithms, high performance computing, modeling and simulation with applications in Sciences, Engineering...

Available to graduate degree candidates in participating departments who have selected an independent research project in which there is a significant computational component.

#### M.S. Course requirements:

9 hours (> grades B or higher) of Computational Science Electives including at least 3 hours outside home department and must attain degree

#### Ph.D. Course requirements:

12 hours (> grades B or higher) of Computational Science Electives including at least 6 hours outside home department and must attain degree

# **Expand degree programs centering on Computational Science**

Currently, we have a Computational Engineering M.S. & Ph.D. Program.

#### Goals for the future:

**Computational Mathematics graduate programs Computational Biology / Bioinformatics graduate programs** 



#### Recent funded and pending proposals

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Sponsor	Title of Project	Amount	Personnel (PI)	Status
US Department of Army (ARMY) (DOD)	Molecular Packing Software for Ad-Initio Crystal Structure and Density Predictions	\$17,474	Seong-Gon Kim	Awarded
(505)	and Benony Fredictions			(03/24/03-12/31/06)
ABSL Power Solutions, Inc.	Portable Energy Divisions: Composites, Modeling, and Integration, Task 2	\$209,990	Mark Novotny	Awarded
				(04/11/06-04/10/07)
Rensselaer Polytechnic Institute	Non equilibrium Growth Phenomena and Scalability in Synchronized Computing Networks	\$274,970	Mark Novotny	Awarded
				(09/01/04-08/31/08)
National Science Foundation	The Seventh Mississippi State-UAB Conference on Differential Equations and Computational Simulations	\$32,000	Hyeona Lim, Ratnasingham Shivaji	Awarded
				(08/15/07-07/31/08)
DOE	Nuclei at Extreme Conditions: A Relativistic Study (Ran through Physics with Overhead split between CCS and Physics)	\$212,000	Anatolijs Afanasjevs	Awarded
				(12/15/06-11/14/09)
Environment Canada	Changepoint Estimation for Canadian Sky-Cloudiness Frequencies Using a Temporal Continuation-Ratio Logit Model	\$20,000	Q. Lu	Awarded
				(12/01/08-03/31/09)
US Department of Defense (DOD)	Molecular Modeling to Develop Better Reactivators (Ran through Center for Environmental Health Sciences	\$48,900.00	Steven Gwaltney	Awarded
(565)	(CEHS) with Overhead split between CCS and CEHS)			(1/11/07 – 1/10/10)
National Science Foundation	Collaborative Research : The role of isolation in species diversification : insights into disperal and evolution of endemics Lotus from the California	\$99,777	Lisa E.Wallace	Awarded
				( 03/01/09 – 02/29/12 )
ERDC	Topological Features and Dynamics of Gene Flow Networks	\$110,000	C. Brooks	Awarded
				(03/02/09-09/30/2011)
MAFES/MS Soybean Promotion Board	Development of a Rapid Genetic Field Race Test for Soybean Cyst Nematode (SCN) and Generation of SCN	\$54,850	V. Klink, G. Lawrence, T. Koger, T. Allen, C. Balbalian	Awarded
Dodiu	Resistance through Gene Inactivation			(04/01/09-03/31/2010)
National Science Foundation	The Eighth Mississippi State- UAB Conference on Differential Equations & Computational Simulations	\$35,000	Hyeona Lim, Ratnasingham Shivaji	Awarded
			,	(06/15/09-05/31/2010)
National Science Foundation	Planning of a Center for Autonomic Computing	\$10,000	I. Banicescu, S, Abdelwahed	Awarded
				(07/01/09-06/30/2010)

### **Recent CCS Proposals**

Sponsor	Title of Project	Amount	Personnel (PI)	Status
DOE	Theory of Coexisting Density Waves in Low Dimensional Quarter-Filled Band Molecular Solids	\$507,111	Torsten Clay	Awarded (09/01/08-08/31/2010)
National Science Foundation	REU site Project: REU in Applied Mathematics and Biostatistics	\$200,000	H.Lim, R. Shivaji,X. Yang, H. Zhang	Awarded (09/15/09 - 08/31/11)
DOE	Nuclei at Extreme Conditions: A Relativistic Study	\$222,000	Anatolijs Afanasjevs	Awarded (11/15/09 - 11/14/12)
MS Soybean Promotion Board	Identifying Full-Length Open Reading Frames of Genes involved in Interactions between Soybean and Nematodes	\$35,000	Vincent Klink	Awarded (12/16/09 – 05/31/13)
ORED (Mississippi State University) (RIP)	Ciliary Dynamics and the Motilities of the Single-Celled Algae Chlamydomonas	\$10,000	Xingzhou Yang	Awarded (1/1/10 - 12/31/10)
ORED (Mississippi State University) (RIP)	Estimation of Latent Class Models with Conditional Dependence Using Multivariate Probit Analysis	\$10,000	Huiping Xu	Awarded (1/1/10 - 12/31/10)
Federal Initiative for Funding (2009-2010)  Department of Defense	Advanced Materials Design for Nano Devices	\$7.02M	R.T.Clay, S.Gwaltney, Seong Gon Kim, H.Lim,M.Novotny, P.C.Ray, R.Shivaji, J.P.Singh, Y.Ki.Hong.	Made it to Authorization bill but not in the Appropriation bill
Federal Initiative for Funding (2010-2011)  Department of Defense	Advanced Materials Design for Nano Devices	\$7.02M	R.T.Clay, S.Gwaltney, Seong Gon Kim, H.Lim,M.Novotny, P.C.Ray, R.Shivaji, J.P.Singh, Y.Ki.Hong.	Pending
Federal Initiative for Funding(2010-2011)  Department of Defense	Towards Reliable and Green Computing Systems: An Automatic Management Approach	\$2,599,651	Ioana Banicescu, Sherif Abdelwahed	Pending

Recent CCS Proposals						
Sponsor	Title of Project	Amount	Personnel (PI)	Status		
US Department of Energy (12/01/08)	Few-and Many-Body Nuclear Theory from QCD	\$383,461	G. Rupak	Pending		
National Science Foundation (01/20/09)	GEPR: Identification of Gene Regulatory Networks Involved in Resistance as Identified by Laser Capture Microdissection and FLX-454 Sequencing of RNA Isolated from Nematode Feeding Sites	\$869,986	V. Klink	Pending		
DOE ( 09/01/09 )	Universality, Nuclear Physics and QCD	\$843,338	G. Rupak	Pending		
National Science Foundation (12/15/09)	Efficient Numerical Methods for Variational Image Restoration and Segmentation	\$217,702	Heyona Lim	Pending		
National Science Foundation (09/30/09)	Composition Markov Chains of Multinomial Type	\$33,165	Haimeng Zhang	Pending		
National Science Foundation (07/24/09)	Collaborative Research: Magnolia grandiFLORA: A digital Herbarium of Collections in Mississippi(Proposal will run through GRI with O/H split 25%/25% between GRI and CCS)	\$677,146	L. Wallace, C. Brooks, G. Ervin	Pending		
NIH ( 09/24/09 )	Early Detection of Myocardial Infraction: A3DDiffusion Tensor MRI Study on Heart Fiber Architecture	\$418,476	Song Zhang	Pending		
National Science Foundation (10/31/09)	Materials Inspired by Network Theory	\$488,960	Mark Novotny	Pending		
National Science Foundation (10/31/09)	Tailoring Magnetic Properties of Hexagonal Ferrites	\$494,638	Seong – Gon Kim	Pending		
National Science Foundation (01/13/10)	A Mechanical and Computational Model of the Unicellular Green Algae Chlamydomonas	\$73,955	Xingzhou Yang	Pending		
National Science Foundation ( 02/01/10)	Characterization of cpDNA SSR's in Lotus for inferring phylogeographic patterns on the Channel Islands	\$14,401	Lisa Wallace	Pending		
National Science Foundation (02/11/10)	UBM Group: The Landscape Genetics of Plant- Pollinator Interactions – Integrating Models and Data	\$237,780	C. Brooks, H. Zhang, L. Wallace, H. Xu, C. Yuan	Pending		
National Science Foundation (03/06/10)	Center for Autonomic Computing at Mississippi State University	\$274,789	I. Banicescu, S. Abdelwahed	Pending		
National Science Foundation (06/01/10)	EMSW21-RTG Research Training in Partial Differential Equations with applications in Biology and Material Science	\$2,126,807	H. Lim, R. Shivaji, X.Yang and S. Yarahmadian	Pending		