2010 Annual Report
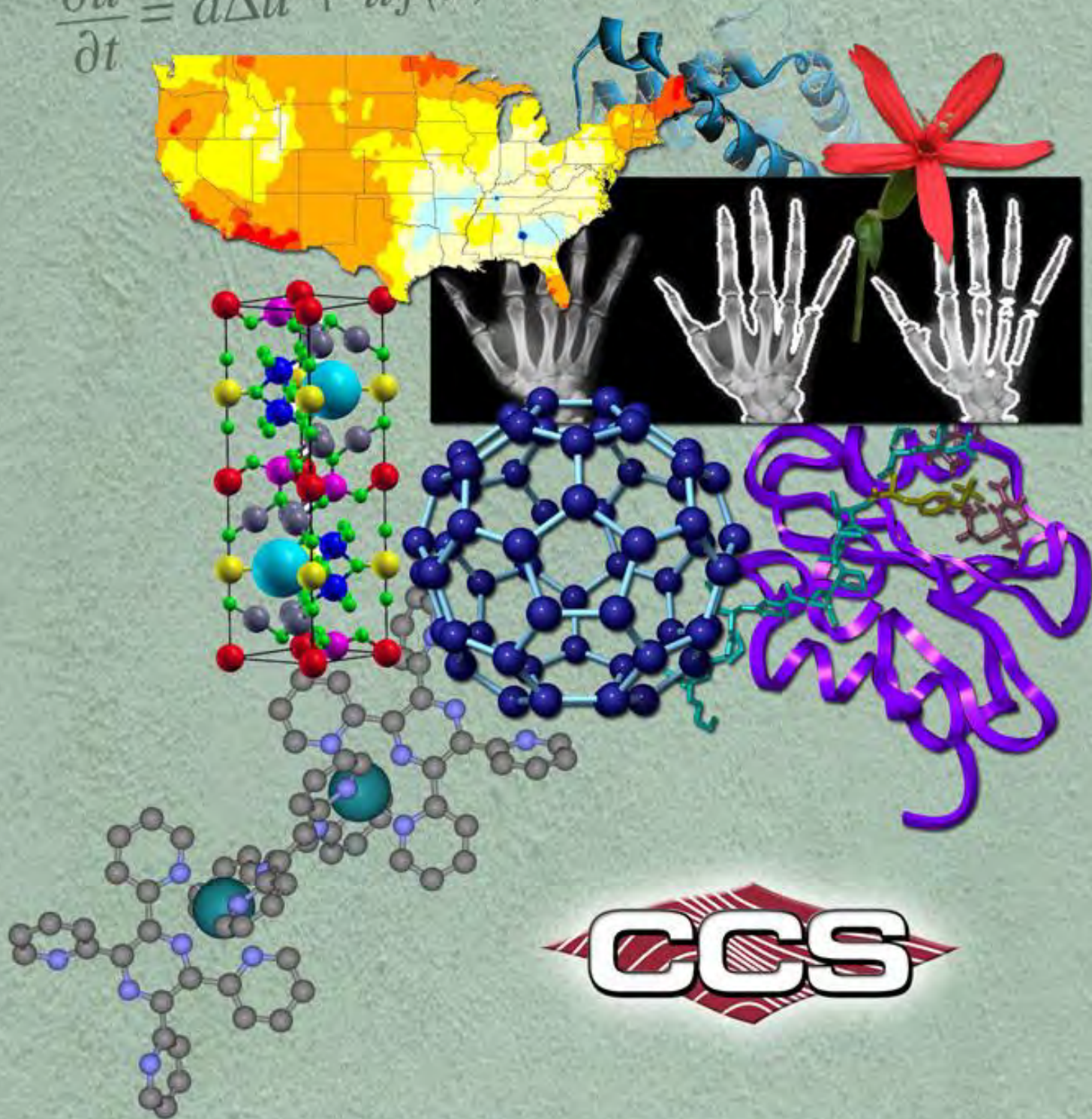## Center for Computational Sciences

$$\frac{\partial u}{\partial t} = d\Delta u + uf(x, u) - c(x)h(x)$$

CCS

Director's Note

The Center for Computational Sciences (CCS) at Mississippi State University is a College of Arts and Sciences center with a mission to foster interdisciplinary research in both the fundamental understanding of and application of all natural sciences. In particular, to model and develop integrated computational environments and crosscutting tools that allows a comprehensive, cross-disciplinary approach to problem solving.

Year 2010 major activities/initiatives include: (1) A major Federal Initiative proposal in "Advanced Materials Design for Nano Devices" (Last year this proposal made it through to the authorization bill but at the last minute did not make it to the appropriation bill. This year, we are very hopeful that it will make it all the way to the appropriation bill and be funded; (2) An NSF funded Research Experiences for Undergraduates (REU) Site in Applied Mathematics and Biostatistics; (3) An open forum for all the researchers interested in conducting research in magnetic material for nanoelectronics; (4) Establishment of a Center for Autonomic Computing; (5) An NSF Proposal for Nanoelectronics 2010 and beyond (NEB) proposal; and (6) Mini Workshop on Mathematical Biology & Computational Modeling. Major events/proposals already planned in the near future include: (1) Major Upcoming Conference: Differential Equation Weekend Conference; (2) Ninth Mississippi State - UAB Conference on Differential Equations and Computational Simulations; and (3) An NSF Proposal for Interdisciplinary Training for Undergraduates in Biological and Mathematical Sciences.

This report will provide details of these activities/initiatives, the list of CCS Personnel, the recent awards and recognitions, and the 2009 & 2010 research publications. Also included in the report are the details on funding activity. Here we have listed the activity from year 2003 onwards to demonstrate the much enhanced activities in recent years. Overall, 2010 has been a successful year for CCS. We look forward to building on this platform, to achieve greater excellence in the very near future.

Ratnasingham Shivaji
W. L. Giles Distinguished Professor
Director, Center for Computational Sciences
Department of Mathematics and Statistics
Mississippi State University

Mathematics
Ratnasingham Shivaji, *Director, W.L. Giles Distinguished Professor*
Hyeona Lim, *Associate Professor*
Seth Oppenheimer, *Professor*
Xingzhou Yang, *Assistant Professor*
Shantia Yarahmadian, *Assistant Professor*

Physics
Seong-Gon Kim, *Associate Director, Associate Professor*
Anatoli Afanasjev, *Professor*
Torsten Clay, *Associate Professor*
Mark Novotny, *Professor and Department Head*
Gautam Rupak, *Assistant Professor*
Dipankgar Dutta, *Assistant Professor*
Matthew J. Berg, *Assistant Professor*

Electrical & Computer Engineering
Sherif Abdelwahed, *Assistant Professor*
Yaroslav Koshka, *Associate Professor*

Biological Sciences
Christopher Brooks, *Assistant Professor*
Diana C. Outlaw, *Assistant Professor*
Vincent Klink, *Assistant Professor*
Lisa Wallace, *Assistant Professor*
Mark Welch, *Assistant Professor*

Industrial Engineering
Mingzhou Jin, *Associate Professor*

Chemistry
Steven Gwaltney, *Associate Professor*

Computer Science
Ioana Banicescu, *Professor*
Changhe Yuan, *Assistant Professor*
Song Zhang, *Assistant Professor*

Statistics
QiQi Lu, *Associate Professor*
Haimeng Zhang, *Associate Professor*
Meng Zhao, *Assistant Professor*

College of Veterinary Medicine, Basic Sciences
Henry X.-F. Wan, *Assistant Professor*

Affiliated Faculty
Edwin A. Lewis, *Professor and Department Head, Department of Chemistry*
Yang Ki Hong, *Professor & E. A. Larry Drummond Endowed Chair of Computer Engineering, Dept. of Electrical & Computer Engineering, University of Alabama*
**Jagadish P. Singh**, *Research Professor, Institute of Clean Energy and Technology*

CCS Current Major Initiative #1

CCS submits a major Federal Initiative proposal in "Advanced Materials Design for Nano Devices"

Dr. Seong-Gon Kim (PI) along with Dr. Ratnasingham Shivaji, Dr. Torsten Clay, Dr. Steven Gwaltney, Dr. Mark Novotny, Dr. Hyeona Lim, Dr. Jagadish Singh and Dr. Yaroslav Koshka submitted a major proposal entitled "Advanced Materials Design for Nano Devices" for Federal Initiative funding from the Department of Defense. Last year this proposal made it to the Authorization bill. We expect the proposal to make it all the way to the Appropriation bill this year.

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 the Sensor and Electron Devices Directorate (SEDD) at the U.S. Army Research Laboratory (ARL).
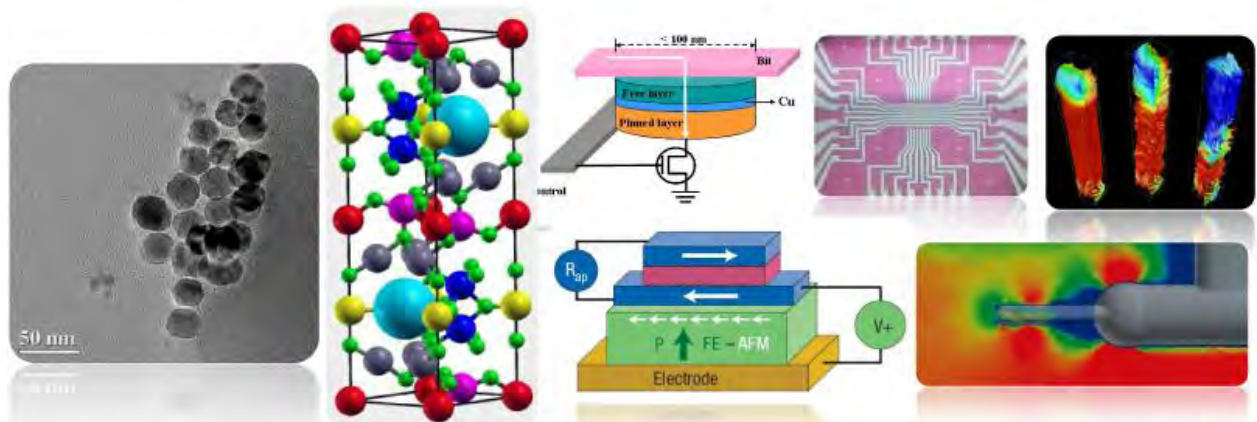

MAIN DELIVERABLES:
1) High-magnetization Ba-hexaferrite magnetic nanoparticles and films
2) Prototype 8x8 arrays of current-rewritable magnetic nanoscale memory cells
3) Prototype 8x8 arrays of voltage-rewritable multiferroic memory cells
4) Gold nanoparticle-based portable sensors for toxic organophosphorus agents

TASKS

Task 1: Tailoring Magnetic Properties of Hexaferrites

Member: S. Kim (Lead, MSU, Phys), T. Clay (MSU, Phys), S. Gwaltney (MSU, Chem), Y. Hong (UA, Elect. & Comp. Eng.)

Goal: To understand the mechanisms of magnetization and magnetoelectric coupling in hexaferrites and optimize these properties for spintronic and multiferroic magnetic memory applications.
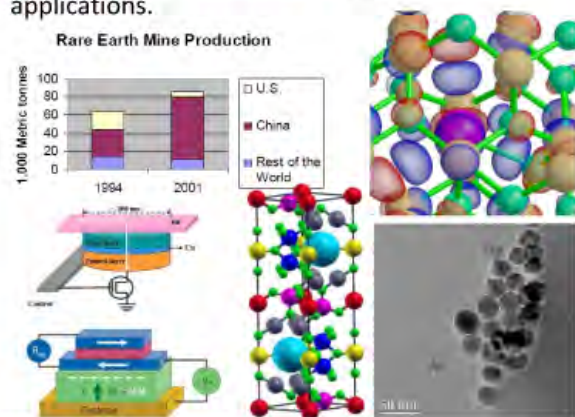
Task 2: Current-Rewritable Magnetic Nanoscale Memory Cells

Member: M. Novotny (Lead, MSU, Phys), H. Lim (MSU, Math), R. Shivaji (MSU, Math), Y. Hong (UA, Elect. & Comp. Eng.)

Goal: To develop current-rewritable, low-power consumption memory cells using a vortex spin-flipping arrangement for nanoscale non-volatile magnetic memory cells.
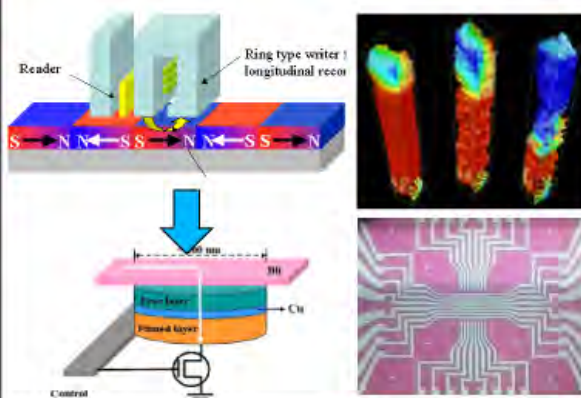
Task 3: Voltage-Rewritable Multiferroic Memory Cells

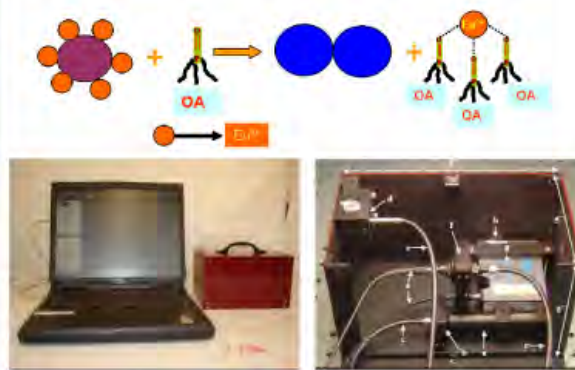**Member:** T. Clay (Lead, MSU, Phys), S. Kim (MSU, Phys), Y. Hong (UA, ECE)

Goal: To develop voltage-rewritable non-volatile magnetoelectric random access memory (MERAM) cells operating at room temperature using multiferroic materials.
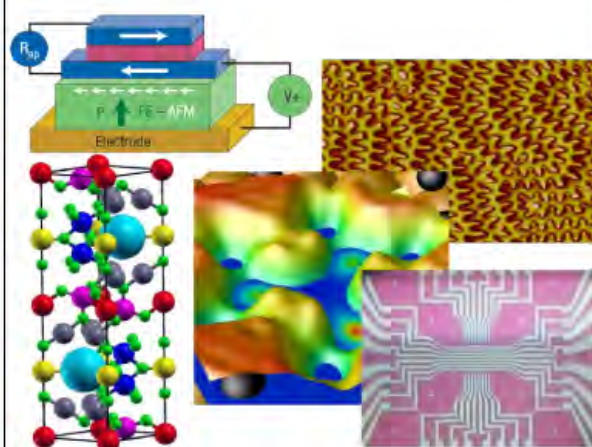
Task 4: Nanosensors for Chemical Warfare Agents

Member: J. Singh (Lead, MSU, ICET), S. Gwaltney (MSU, Chem), P. Ray (JSU, Chem), F. Yueh (MSU, ICET)

Goal: Develop a battery operated state-of-the-art, cost effective, compact, high sensitivity and specificity nanoparticle based surface energy transfer (NSET) and surface enhanced Raman spectroscopy (SERS) nanosensors for chemical warfare agents.

ORGANIZATION

	Advanced Materials Design for Nano Devices		Administration	
	PI: Seong-Gon Kim (MSU, Phys)		R. Shivaji (CCS Director, Math)	

	Task 1	Task 2	Task 3	Task 4
Title	Tailoring Magnetic Properties of Hexaferrites	Voltage-Switching Multiferroic Memory Cells	SiC Nanostructures for Spintronics and Biosensors	Nanosensors for Chemical Warfare Agents
Lead	T. Clay (MSU, Phys)	M. Novotny (MSU, Phys)	Y. Koshka (MSU, ECE)	J. Singh (MSU, ICET)
Team	S. Kim (MSU, Phys) S. Gwaltney (MSU, Chem) Y. Hong (UA, ECE) S. Erwin (NRL)	S. Kim (MSU, Phys) T. Clay (MSU, Phys) H. Lim (MSU, Math) Y. Hong (UA, ECE)	S. Kim (MSU, Phys) R. Shivaji (MSU, Math) Y. Hong (UA, ECE)	S. Gwaltney (MSU, Chem) P. Ray (JSU, Chem) F. Yueh (MSU, ICET)
Postdoc	2 Postdoc	3 Postdoc	2 Postdoc	1 Postdoc
Student	3 GRA	6 GRA	2 GRA	4 GRA

Interdisciplinary team: **11 faculty**, **3 research associates**, and **8 postdocs** in Computational Physics, Experimental Physics, Chemistry, Mathematics, Electrical and Computer Engineering, and Materials Science
Education: **15 doctoral students and 8 postdocs** will be involved in research each year

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;
  ▪ SemiSouth, Starkville, MS;
  ▪ Custom Sensors & Technology, Frenton, MO.

COLLABORATION WITH FEDERAL AGENCY

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

...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. 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 ... I must add that we are also very impressed with Center for Computational Sciences facilities at MSU. This was the reason ARL has awarded initial funding of $15,392 to start the work.

I congratulate you and your colleagues on together...

$15,392 Seed funding (Jul 2010)

EXPANDING MSU CAPABILITIES

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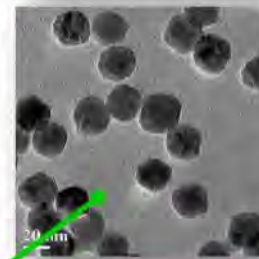

Science 273, 483 (1996) – Crystalline ropes of carbon nanotubes (S. Kim with Nobel laureate R. Smalley)

Micromagnetc simulation (M. Novotny)
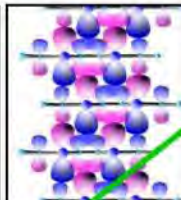
Superconductivity (R. T. Clay)

❑ 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 $Ni_{80}Fe_{20}$ thin film elements
  ▪ Recently synthesized world's smallest (< 20 nm) spherical Ba-hexaferrite nanoparticles.
❑ Dr. S. Erwin of NRL (Task 1) is one of the world's best experts in nanocrystal doping and theory of magnetism.
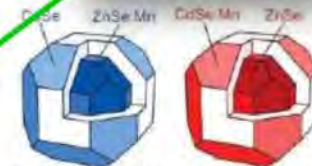
Erwin, et al., "Doping Semiconductor Nanocrystals," Nature 436, 91 (2005)

CCS Received National Science Foundation funding to host a site for a 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. The REU site project for 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 modeling in biostatistics.

Report on the 2010 NSF REU Site in Applied Mathematics and Biostatistics

May 30 - August 7, 2010

Hosts: The Center for Computational Sciences & the Department of Mathematics & Statistics, College of Arts & Sciences, Mississippi State University.

Faculty Mentors: Hyeona Lim (PI), Ratnasingham Shivaji (Co-PI),

Xingzhou Yang & Heimeng Zhang.

Graduate Student Mentors: Dagny Grillis, Jerome Goddard II & Arundhati Bagchi Misra.

Application and Recruitment Process:

The 2010 REU program targeted undergraduate US citizens and permanent residents who completed their sophomore or junior year by the end of Spring 2010. Students who have background in multivariable calculus, linear algebra, and ordinary differential equations or probability prior to the start of the REU program were eligible to apply. Women, students from other underrepresented groups, community college students, and students from regions and institutions with limited research opportunities were actively recruited and encouraged to participate. The application deadline was February 15, 2010.

The selection of the participants was based on their academic performance, their aptitude in mathematical sciences, and recommendations. Of the seventy-one applications received, the following seven students were selected:

John Corring, University of Southern Mississippi
Justin Hansen, University of Vermont
Bonnie Roberson, Mississippi State University
Brittany Stephenson, Mississippi State University

Helene Duke, Providence College
Emily Poole, University of Arkansas
Yicong Yong, University of Florida

Research and Education Activities:

The objectives of this 10-week REU site program were to involve the participating students in meaningful research activities, to show the students the enjoyment of doing research, to encourage them to pursue advanced degrees in mathematical sciences, and to increase the participation in research activities by women and other underrepresented groups.

There were four groups working on four different research areas: Image Processing (mentor: Hyeona Lim, graduate student mentor: Arundhati Bagchi Misra, participants: John Corring, Helene Duke), Population Dynamics (mentor: Ratnasingham Shivaji, graduate student mentors: Jerome Goddard II, Dagny Grillis, participants: Emily Poole, Bonnie Roberson, Brittany Stephenson), Computational Mathematical Biology (mentor: Xingzhou Yang, participant: Yicong Yong), Highly Stratified Model in Biostatistics (mentor: Haimeng Zhang, participant: Justin Hansen). There were activities to improve the participants' written and oral presentation skills as well as computational skills. By closely working with a team of four faculty members and three doctoral-level graduate students, the participating undergraduate students had the opportunity to perform research in a Ph.D. Granting department/interdisciplinary research center, gain insight into the roles and responsibilities of active researchers, discuss graduate school choices, and be in an active research environment. All four groups have developed new methods and findings for their projects.

We also invited five colloquium speakers (3 in academia and 2 in industry) from different disciplines. The following is a list of speakers and their title of talks:

1. Seong-Gon Kim, Department of Physics and Astronomy, MSU, June 25. Title: Ranking Billions of Web Pages Using Diodes: How Google works and how to beat it
2. Michael Neumann, Department of Mathematics and Statistics, MSU, July 8. Title: The fundamental theorem for finite Markov chains revisited
3. Chris Brooks, Department of Biological Sciences, MSU, July 13. Title: Using graphs to model biological invasions
4. Lalitha Venkataramanan, Schlumberger Doll Research, July 22. Title: Research in applied mathematics at Schlumberger
5. Stan Dickens, Southern Farm Bureau Life Insurance Company, July 28. Title: Pursuing a career in the actuarial field
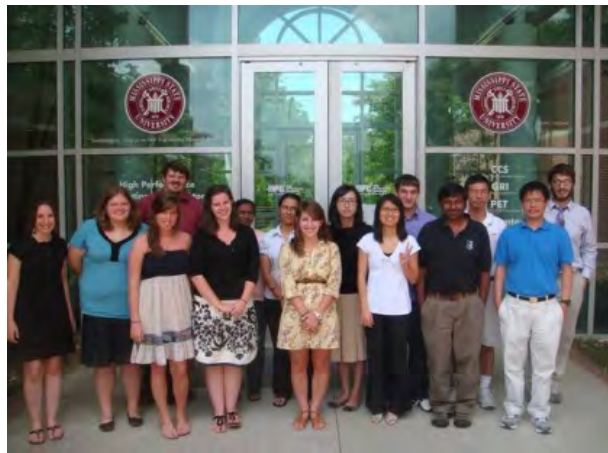
We had two educational trips. On Friday, July 9, we visited the Department of Mechanical Engineering at the University of Alabama at Birmingham, where the participants listened to presentations on Computational Fluid Dynamics, Computational Geometry/Visualization, and Computational Methods in Impact Engineering: Finite Element Method and Multibody Dynamics and their Applications. On July 26-27, we visited the Department of Mathematics at Tulane University. The Tulane faculty presented the following three lectures to our REU students:

An interesting sequence coming from an integral (by Victor Moll)
Mathematics and the modeling of swimming microorganisms (by Lisa Fauci)
A gambler's ruin is a random walk (by Ricardo Cortez).

We also had several social activities such as movie nights, frequent coffee hours, and lunch and dinner meetings. We had a joint picnic with the REU group in the Department of Computer Science and Engineering on August 1.

Findings:

For Image Processing project, new partial differential equation (PDE)-based denoising models which are modified Euler-Lagrange equations derived from noise constrained functional minimization problems were developed. These PDE models are designed to rectify speckle noise present in ultrasound images. Non-standard numerical schemes of the corresponding speckle denoising models were derived and stability of the new schemes was also analyzed. Numerical results from a variety of computational strategies and models for ultrasound images were compared.

For Population Dynamics project, a one-dimensional reaction-diffusion model arising in population dynamics where the per capita growth rate is a weak Allee type was studied. In particular, the effects of grazing on the steady states were considered and the complete evolution of the bifurcation curve of positive solutions as the grazing parameter varies was discussed. The results were obtained via the quadrature method and Mathematica computations. In particular, it was established that the bifurcation curve is S-shaped for certain ranges of the grazing parameter. This occurrence of an S-shaped bifurcation curve was also proven analytically.

For Computational Mathematical Biology project, a computational model to understand the particle dynamics around the choanoflagellates was considered. The flow patterns were shown by visualizing how the flagellum, microvilli, suspended particles interact with the surrounding fluid. The regularized Stokeslets method, a grid free method, was used to solve the governing equations. The Runge-Kutta method was employed to solve the related ODE system. The numerical results were compared with the data in the published biological experiments.

For Highly Stratified Model in Biostatistics project, the efficiency of the MPLE for nested case-control sampling under the highly stratified situation was considered, where the covariate values are increasingly less dependent upon the past and there is no censoring. In particular, through numerical study under the parametric distribution for the failure time, the efficiency of the MPLE was investigated and its performance was compared with the MLE when the sample size is finite.

Research Presentations and Publications:

On Thursday, July 29, all 4 groups gave a poster presentation at the Summer 2010 Undergraduate Research Symposium which was hosted by the Shackouls Honors College at Mississippi State University. Two students from the population dynamics group gave presentations at the 30th Southeastern-Atlantic Regional Conference on Differential Equations in October 1-2, 2010. One student from the image processing group gave a talk at the Northeastern Section of the Mathematical Association of America 55th Annual Fall Meeting in November 19, 2010. Also students from all four research groups presented their results at the 2011 Annual American Mathematical Society meeting in New Orleans in January 6- 9. Further, three students participated in the 13th Nebraska Conference for Undergraduate Women in Mathematics held in January 28-30, 2011 and gave presentations. The population dynamics group has already submitted their results for publication in the journal INVOLVE. The other groups are currently preparing manuscripts for submission.
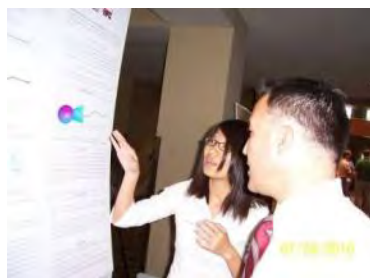
Training and Development:

The first two weeks were spent as an orientation and training period. 3 Ph.D. students gave lectures on basics of MATLAB, Mathematica, Metric Spaces, and LaTeX. These graduate students helped the mentors to guide the REU participants so that they can have the opportunity to perform research on their projects.

Outreach Activities:

The website for our REU program has been created (http://math.msstate.edu/events/reu) and it is open to the public. In the fall semester after the 2011 REU program, we plan to conduct a one-day Research Experiences for Teachers (RET) workshop for teachers from neighboring high schools. We will invite teachers and have a workshop to disseminate new findings from the REU program and help them to have their students prepare for undergraduate research.

Contributions to Human Resource Development:

Among the 7 participants we selected this year, 5 were women. Also, 2 out of 3 graduate student mentors were women. We will continue to make every effort to reach out to women and other underrepresented groups and encourage their participation.

Evaluations:

Overall rating given by the students: 4.7/5

Extracts from REU participants' comments:

The mentoring and guidance in this specific program were amazing and a lot was learned during research in highly stratified models in biostatistics. I learned how to carry out research on my own as well as worked closely with my faculty advisor. The research in general was very informative and taught me a lot.

The graduate mentors, faculty mentor, and fellow students in my research group were amazing. I have no complaints about any of these people. I worked very closely with my mentors, but we were also able to do our own research.

My mentor is a fantastic advisor, and I really learned a lot from him this summer. He challenged me and the research was difficult, but he also made sure I did not feel overwhelmed or incapable. The graduate mentors were also a really big help- it was fun to work with them and they did a great job. I enjoyed the laid back structure our group had for meetings and meeting times. I'm looking forward to working with my mentor more in the fall.

My mentor gave me very effective instructions every time we met and I was able to do some research on my own following his directions and hints. This program definitely has trained me how to do independent research.

My mentor was amazing. His vast knowledge related to this area of study made our research run a lot more smoothly. He guided us down all the right paths anytime we were stuck or frustrated and always knew how to lead us in other directions to obtain different results. He ensured our research was thorough and accurate and compelled us to check all of our work. The graduate mentors were also an immense help. Any problems with proofreading, from things such as our paper to codes in Mathematica, they could solve. They were always willing to meet with us at any time and help us in any way possible, including over the phone when they weren't available in person. My mentor did a great job of giving us a very limited amount of information to start with and forcing us to work independently to obtain results. He has done so so well that I now find myself asking new questions and coming up with new ideas to research.

The application process seemed very efficient. It was short enough that it did not seem tedious and overdone, but it was also long enough to receive what I feel was all the necessary information about each applicant.

I'd suggest playing up the facilities- I had no idea the caliber of research centers Mississippi State had until I arrived in Starkville. I think information about HPCC and all that goes on there would really increase the pool.

I am way beyond satisfied with the stipend and other benefits. The advisors outdid themselves. We always felt welcomed and very well taken care of. Honestly, we often felt very spoiled. It was very well planned and very well carried out.

Really good benefits- we were well taken care of throughout the program. I really enjoyed the variety of colloquium speakers, and the fieldtrips were fun as well. Herbert was clean and a

decent size room, but it might be better to put next years participants in the newer dorms if possible. Also, maybe more social activities at the beginning of the summer

The entire research program was awesome. There was nothing that should be changed. My only suggestion would be to move the social activity with the other REU students to an earlier date. This would give the students time to make friends with the other students earlier.

Before this program, I did not even know what research in mathematics entailed. I now know how to take one simple differential equation and study it incredibly thoroughly. I now also feel very, very comfortable using Mathematica; whereas, before my knowledge in that area was also limited. Another invaluable skill I gained is the use of LaTex to write mathematics papers. I am very excited to now know how to do this. Furthermore, I gained knowledge on myself and how to manage my time and stop procrastinating. I find myself more motivated to complete tasks since I do not know what the results may be.

The program has changed my entire view of mathematics. It has also helped me realize what I may want to do with my mathematics major in the future. It helped a lot to be around graduate students because I may want to follow in their footsteps, and it was nice to see firsthand what that may be like. I used to be somewhat nervous about being a math major because I had no idea what I wanted to do, but at this point I feel very confident in my decision to stick with this major. This program has helped me to love it more.

This program has taught me lots of skills that I can use right now for my studies, such as latex and matlab. Since I have some taste of what real research is like, in the future, I will be ready for any difficulty that I will face when doing research.

My REU experience has confirmed that I want to continue my mathematical studies on the graduate level. I think I learned a lot about challenging myself academically, and how to push through frustration to achieve a rewarding result.

This program has taught me about future studies and what is required in grad school. It has thus given me a step forward in this area as well.

Scientists, Mathematicians, and Engineers join to provide an open forum for all the researchers interested in conducting research in magnetic material for nanoelectronics.

Purpose:

To provide an open forum for all researchers at Mississippi State University interested in conducting research in **magnetic materials for nanoelectronics**:

- to learn about the latest and emerging development in the field;
- to facilitate the sharing of new ideas;
- to permit the maximum utilization of shared resources;
- to promote collaboration among members for research and external grant application.

Members:

- Seong-Gon Kim (Chair) – Physics and Astronomy, CCS
- Mark Novotny – Physics and Astronomy, CCS
- Torsten Clay – Physics and Astronomy, CCS
- Yaroslav Koshka – Electrical and Computer Engineering
- Steve Gwaltney – Chemistry, CCS
- Jagdish Singh – ICET
- Ratnasingham Shivaji – Mathematics, CCS
- Hyeona Lim – Mathematics, CCS
- Xingzhou Yang – Mathematics, CCS
- Sungho Kim – CAVS
- Amitava Moitra -- CAVS
- And more ...

Format:

❏Monthly meetings
- ❖ A lunch meeting will be held once each month during the academic year (4 times a semester).
- ❖ One or two persons will give short presentations (typically 20-30 minutes) on their research or new ideas for collaboration.
- ❖ Discussions on the topic related to the speaker's research or proposed ideas.

❏Special Seminar Series
- ❖ One special seminar will be held in each semester.
- ❖ An external speaker with national or international recognition in the field will be invited to present his/her research and review the latest developments.
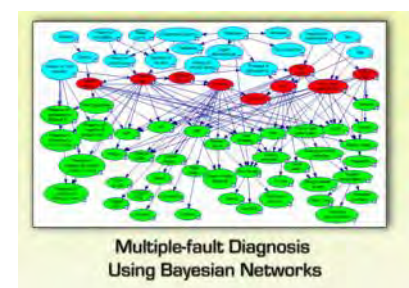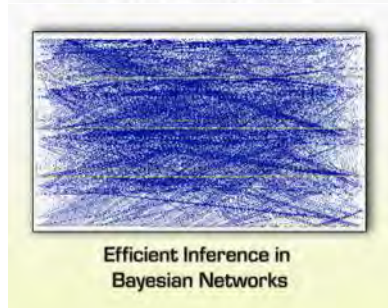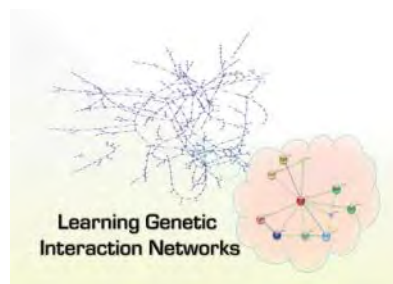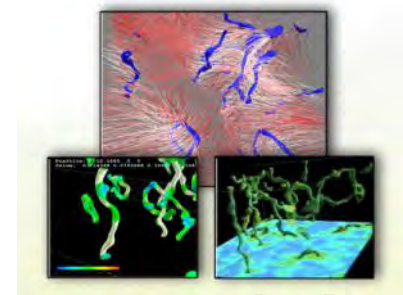- ❖ Dinner will be served to all participants.

Support:

- ❖ ORED -- $2,000 per year
- ❖ CCS -- $1,200 per year
- ❖ Total -- $3,200 per year

Computer scientists and engineers join to establish a Center for Autonomic Computing

CCS is pleased to announce that **Dr. Ioana Banicescu** (PI) **and Dr. Sherif Abdelwahed** (co-PI) received a National Science Foundation (NSF) award (2010-2015) for establishing a new Center for Autonomic Computing (CAC) site at Mississippi State University (MSU), the first NSF Industry-University Cooperative Research Center (I/UCRC) ever established at MSU. This new center site joins the NSF CAC initiated in 2008 by a consortium of three universities: University of Florida, University of Arizona, and Rutgers University. The NSF CAC is funded by the NSF I/UCRC program of the National Science Foundation, CAC members from industry, government laboratories, and university matching funds.

   The CAC at MSU brings to the existing NSF CAC much needed complimentary capabilities in the areas of model-based autonomic computing, and resource management and scheduling in parallel and distributed systems, representing the main areas of expertise of both Dr. Ioana Banicescu and Dr. Sherif Abdelwahed. Therefore, the CAC at MSU is expected to be successful in extending these new capabilities of the emerging technology of autonomic computing to systems and applications in various areas of science and engineering. Other CCS faculty with high potential for affiliation with CAC are Dr. Song Zhang, and Dr. Changhe Yuan. Following are a few NSF CAC highlights describing characteristics at each of its sites (including the CAC at MSU site) in terms of: goals, collaborations, technical scope of industry-university projects, activities for faculty and students, benefits of membership for collaborators from industry and government laboratories.

Model-based Self-managing Systems

Control-based Framework for Self-managing Systems

Learning Genetic Interaction Networks

Efficient Inference in Bayesian Networks

Multiple-fault Diagnosis Using Bayesian Networks

GOALS OF THE CENTER

- To function as a multidisciplinary center of excellence in autonomic computing research fostering long-term collaborative partnerships amongst industry, academe, and government;
- To discover, share and leverage synergies of concepts, technologies and resources needed by industry-relevant autonomic computing research in collaboration with CAC partners;
- To educate a diverse body of students on the interdisciplinary field of autonomic computing;
- To accelerate the creation and transfer of knowledge and technology for autonomic computing into industry and commercial products.

BENEFITS OF MEMBERSHIP

CAC supporting members are afforded access to leading-edge developments in autonomic computing and to knowledge accumulated by academic researchers, government laboratories researchers, and other industry partners. For each of the participant center sites, new members will join a growing list of founding members. The NSF CAC currently includes the following members: Citrix, the US Army Corps of Engineers Engineer Research and Development Center (ERDC), Intel, Microsoft, Raytheon, Xerox, Imaginestics, Avirtec, MobiLaps, and others. Benefits of membership include:

- Collaboration with faculty, graduate students, post-doctoral researchers and other center partners;
- Choice of project topics to be funded by members' own contributions;
- Formal periodic project reviews along with continuous informal interaction and timely access to reports, papers and intellectual property generated by the center;
- Access to unique world-class equipment, facilities, and other CAC infrastructure;
- Recruitment opportunities among excellent graduate students;
- Leveraging of investments, projects and activities by all CAC members;
- Professional networking with new partners for competitive funding opportunities.

TECHNICAL SCOPE

Autonomic computing (AC) denotes a broad area of scientific and engineering research on methods, architectures and technologies for the design, implementation, integration and evaluation of special- and general-purpose computing systems, components and applications that are capable of autonomously achieving desired behaviors. AC systems use self-management techniques to enable independent operation, minimize cost and risk, accommodate complexity and uncertainty, or command systems of systems with large numbers of components. Hence, system integration and automation of management are important areas of research whose contexts subsume other AC research topics.

These might include, to varying degrees, self-organization, self-healing, self-optimization (e.g., for power or speed), self-protection and other so-called self-* behaviors. CAC research activities involve several disciplines that impact the specification, design, engineering and integration of autonomic computing and information processing systems. These include design and evaluation methods, algorithms, architectures, information processing, software, mathematical foundations and benchmarks for autonomic systems and applications. Solutions devised through CAC research are applicable to multiple levels of both centralized and distributed systems and applications. Collectively, the CAC universities have research and education programs whose

strengths cover the technical areas of the center. Within this broad scope, the specific research activities will vary over time to adapt to the needs of each center members and the evolution of the field of autonomic computing.

PERSONNEL
Research at the CAC universities is undertaken by faculty, graduate students, and post-doctoral researchers from multiple disciplines including computer science, computer engineering, electrical engineering, and others. Industry and government partners are welcome to have researchers in residence at the Center or as temporary visitors to campus making use of its facilities.

FACILITIES
Major existing facilities in the advanced computing and information systems research labs at University of Florida, University of Arizona, Rutgers University and MSU support the operation of the NSF CAC center. At present, facilities include cutting-edge computer systems and software infrastructure mirroring state-of-the-art capabilities found in industry settings. CAC resources are locally and externally connected via high-speed networks. Deployment of a distributed, shared instrumented testbed for center-wide experimental research on cross-layer data center autonomics is currently underway.

OTHER HIGHLIGHTS
CAC at MSU had a successful participation with a number of projects at the biannual NSF CAC review meeting at the University of Florida on October 4-6, 2010, and is presently preparing to participate with a number of projects and proposals to the next biannual review, in April 4-6, 2011, at Xerox ACS in Dallas.
Four PhD students are currently participating in the CAC at MSU, and gave talks and presented posters on the funded and proposed projects. The CAC at MSU has a strong collaborator at Vanderbilt University with Dr. Abhishek Dubey, who is an active participant in the MSU projects.
    A number of proposals for continuing support of the center have been submitted to NSF. Moreover, a number of papers describing the ongoing collaborative work within the center have been submitted, accepted or awaiting publications in peer review venues (journals and conference proceedings). Recently, both Dr. Ioana Banicescu and Dr. Sherif Abdelwahed received the following awards: the Bagley College of Engineering Hearing Faculty Excellence Award, and the MSU State Pride Award.
    For additional information, visit the NSF CAC page at http://www.nsfcac.org and our NSF CAC at MSU page at http://www.nsfcac.msstate.edu

CCS Current Major Initiative #5

National Science Foundation (NSF) Proposal:
Nanoelectronics for 2010 and beyond (NEB) proposal.

Title: Voltage-switching non-volatile magnetoelectric random access memory (MERAM) cells operating at room temperature based on multiferroic hexaferrites

Team: Seong-Gon Kim (Phys), Mark Novotny (Phys), Yaroslav Koshka (ECE), Yang-Ki Hong (ECE, UA)
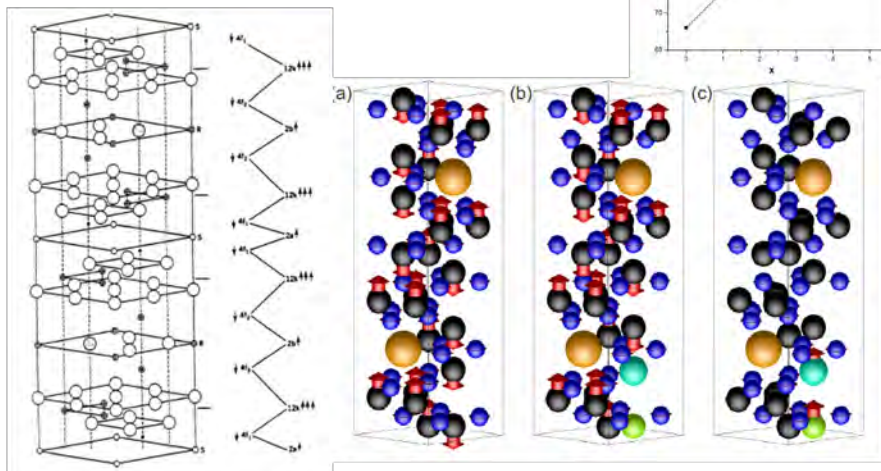
Goal: To develop a non-volatile magnetoelectric random access memory (MERAM) cell operating at room temperature based on multiferroic hexaferrites whose logic state (0 or 1) can be switched by an applied voltage.

❖ NSF proposal – "Voltage-switching non-volatile magnetoelectric random access memory (MERAM) cells operating at room temperature based on multiferroic hexaferrites," PI: Seong-Gon Kim, co-PIs: Mark Novotny, Yaroslav Koshka, Yang-Ki Hong (Univ. of Alabama); Selected by ORED (ORED award #530111) to represent MSU for the full proposal, submitted on Jan. 19, 2011

Preliminary Results

ZnSn-substituted Sr-hexaferrite $SrFe_{12-x}(Sn_{0.5}Zn_{0.5})_xO_{19}$ => Enhancement of saturation magnetization

Morisako et al, JAP **107**, 09A734 (2010)

Mini Workshop on Mathematical Biology & Computational Modeling

Events/Proposals already planned in the near future include:

[1] *Differential Equations Weekend Conference*

[2] *The 9th Mississippi State-UAB Conference on Differential Equations and Computational Simulations will be held in May 2012 at Mississippi State University.*

The primary objective of these conferences is to provide a common forum for mathematicians, scientists, and engineers from industries, federal laboratories, and academia, where they can exchange research and development ideas. The conference aims to promote research and education in mathematical and computational analysis of theoretical and applied differential equations. This conference centers on the interaction of engineers, physicists, and mathematicians.

Information on previous 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
Theresa Windus, AMES LAB, U.S. Department of Energy, (IA)

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.

For more information contact:
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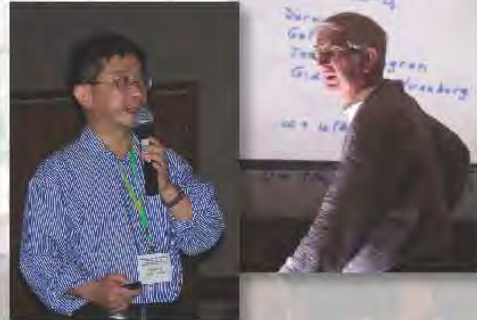
The *Seventh* Mississippi State-UAB Conference on Differential Equations and Computational Simulations
November 1-3, 2007

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 three-day 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* Mississippi State-UAB Conference on Differential Equations and Computational Simulations
May 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 two-day 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 two-day 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.

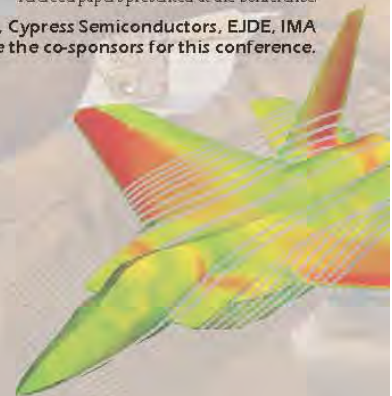**EJDE, IMA and NSF were the primary co-sponsors for this conference.**

The *Fourth* Mississippi State Conference on Differential Equations and Computational 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 two-day 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 two-day 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 two-day 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.

For more information contact:
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Jianping Zhu, jzhu@math.uta.edu · Hyeona Lim, hlim@math.msstate.edu · Roy Koomullil, rkoomul@uab.edu
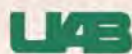
This is to thank you for the great meeting you provided the community of Differential Equations and Computational Simulations. Once more you organized the best meeting in the nation.

<div align="right">

Alfonso Castro, Harvey Mudd College

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The meeting was wonderful. MSU is always amazingly hospitable. I had many useful mathematical discussions with old friends and with new acquaintances.

<div align="right">

Jerry Goldstein, University of Memphis

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The conference was excellently organized; the organizers did a great job. This is my third participation to the MSU-UAB Conference and I consider this event very important for the differential equations and computer simulations people. The organizers came up with a very good choice of plenary speakers and the parallel sessions were populated with many well-known researchers. The social aspect of the conference was also carefully taylored. I think that I speak on behalf of all participants when I say that we all had a great and productive time at the 8th MSU-UAB Conference. I look forward to participate to the 9th MSU_UAB Conference on Differential Equations & Computer Simulations.

<div align="right">

Nicolae Tarfulea, Purdue University Calumet

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This was a great conference, outstanding principal speakers, an environment conducive to scientific exchange and personal interaction, and perfectly organized. Many thanks to the organizers, I really appreciate their effort.

<div align="right">

Georg Hetzer, Auburn University

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It has been one of the best conferences in DEs and DSs that I attended in recent years! I was somewhat reserved and not expecting much going south to Mississippi for the first time. But the reality has exceeded any of my expectations! The organization, the venue, and the logistics were just excellent as were the talks and all the social events. Don't change much for the future conferences, and there is not much to improve or add! Thank you very much for the excellent event!

<div align="right">

Anatoli F. Ivanov, Penn State University

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I can even say it is the best conference I have attended. Organizers take care of almost everything and we just focus on the conference. We did not need to worry about transportation- they pick up back and forth from airport to hotel and from hotel to conference center. We did not need to worry about food-they offer very nice food with lots of choices. The banquet is not only a good dinner but also a wonderful social time.
So we have lots time to focus on the conference and talk to other researchers. I was educated by the wide range topics covered by principal speakers. It is good to learn so many related research areas in differential equations and computational simulations. I like the time slots of principal speakers and parallel sessions. I also like the idea to have a special issue of EJDE for some papers presented in the conference.
At the end, I would like to take this opportunity to thank Dr. Shivaji, Dr. Lim and all other organizers and volunteers. You have done a great job!

<div align="right">

Zhifu Xie, Virginia State University

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[3] *NSF-UBM Proposal*

Biologists, computer scientists, and statisticians are planning to submit an NSF-UBM (National Science Foundation – Interdisciplinary Training for Undergraduates in Biological Sciences and Mathematical Sciences) proposal in the near future.

Dr. Christopher Brooks will lead a team of members, Haimeng Zhang, Lisa Wallace, and Changhe Yuan, in the submission of a UBM Group proposal **"The Landscape Genetics of Plant-Pollinator Interactions-Integrating Models and Data"**.
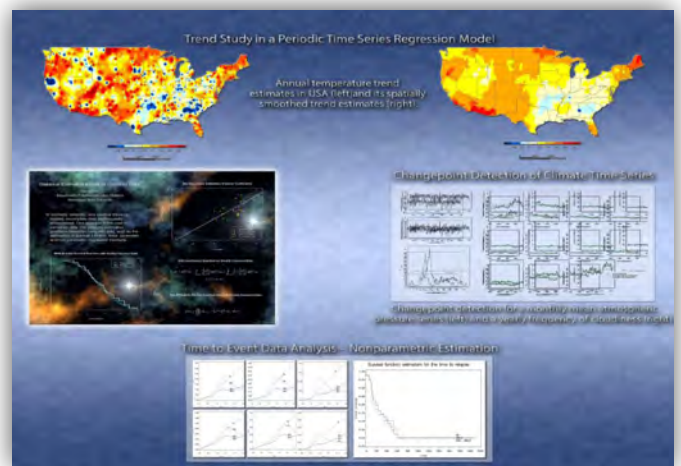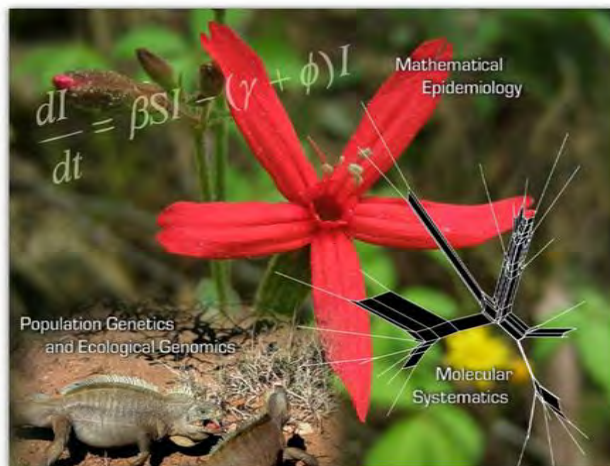
* Such an UBM proposal was submitted in 2009. Though reviews were quite good it was not selected for funding. We plan to resubmit the proposal in the near future.

The UBM Group proposal at Mississippi State University will be a broad effort to provide underrepresented groups in science and mathematics with educational and research opportunities in mathematical biology. This project target students in an anticipated pool of more than 450 enrolling each year across majors whose performance would place them among the top 15% of all students nationally. Students will participate as fellows in the program for three consecutive years, providing them with a comprehensive educational exposure to mathematical biology while involving them in research projects that are addressing important questions in landscape genetics. Each participant will follow a prescribed track of courses depending on their home discipline during the academic year while working 10-15 hours on their research projects. In the summer, students will participate in workshops that are intended to supplement their regular academic training with instruction in the specific skills necessary for their research. Training and research time will encompass approximately 40 hours per week for a ten week period each summer. The goal will be to provide a comprehensive educational experience for students in underrepresented groups and encourage them to pursue careers in math and science.

Intellectual Merits

The proposed project will provide critical information on the mechanisms that influence the movement of genes via pollen dispersal at two critical scales of organization – within and between populations. This information will be especially critical to understanding the role of pollinators in the conservation of orchids as a group. The study organism in this project, *Tipularia discolor*, is a relatively common species in the eastern United States which possesses many important characteristics shared with other rare orchid species throughout the world. Understanding the role that pollinators play in this system will provide a benchmark against which other orchid species can be compared. Not only is this critical to understanding orchid biology, but it is also at the cutting edge of applied mathematics associated with real-world complex networks. Fitting networks to real data and comparing networks derived from different, but similar datasets will be important in the future applications of complexity theory in ecology and evolutionary biology.

Broader Impacts

It is becoming increasingly clear that advancement in the sciences is most efficiently accomplished when hypotheses are well-defined, and when associated assumptions are made explicit. The increasing use of mathematical models in the biological sciences reflects an increasing recognition of their value as scientific hypotheses. Mathematicians and biologists will need to work together to develop appropriate mathematical and biological theories and methods necessary to continue this kind of advancement in both disciplines. This UBM group proposal will improve the involvement of underrepresented groups in these fields while enhancing student interest in pursuing careers at the nexus of these two fields. This project will contribute to that effort by providing a well-rounded experience by integrating education, research and professional development for our students. All PI's have a strong record of involving undergraduate students in research and have demonstrated a commitment to developing an interdisciplinary program in mathematical biology at MSU, including participation in a Math-BioWorkshop held at MSU in 2008, NSF-funded REU programs in Mathematics and Biology, and participation in the Biology Undergraduate Research Program. As the largest degree granting institution for minority students, Mississippi State University is uniquely poised to engage and train minority students in mathematical biology. Additionally, involvement of all levels of academic faculty, graduate students and undergraduate students will provide valuable experiences in mentoring and leadership for the PI's and graduate students and hands-on research experiences for the undergraduates in addition to traditional classroom instruction in mathematics, biology, and new interdisciplinary courses. Students will be expected to present their research design, progress, and results in informal lab meetings and at scientific meetings, in addition to contributing to the publication of manuscripts.

** *The collaboration between the biologist and statistician has already begun due to this proposed CCS project. In fact recently Brook and Zhang publish the following paper:* Brooks, C. and Zhang, H. (2010) A null model of community disassembly effects on vector-borne disease risk. Journal of Theoretical Biology, 264, 866 - 873.

Dr. Christopher Brooks was awarded an ERDC grant for the project "Topological Features and Dynamics of Gene Flow Networks".

Dr. Mark Novotny filed a patent for "System and Method for Charging Rechargeable Batteries".

Dr. Lisa Wallace received a National Science Foundation award for the proposal titled, "Collaborative Research: The role of isolation in species diversification..." which will run till 2012.

Dr. Anatolis Afanasjevs brings a DOE grant for the project titled, "Nuclei at Extreme Conditions: A Relativistic study" which will run till 2012.

Dr. Torsten Clay is an active researcher who has been awarded a DOE grant titled, "Theory of Coexisting Density Waves in Low Dimensional Quarter – Filled Band Molecular Solids" which will run till 2012.

Dr. Qi Qi Lu was awarded a grant from Environment Canada for the project "Changepoint Estimations for Canadian Sky-Cloudiness Frequencies Using a Temporal Continuation-Ratio Logit Model".

Dr. Vincent Klink was awarded a grant from the MS Soybean Promotion Board for the project "Identifying Full-Length Open Reading Frames of Genes involved in Interactions between Soybean and Nematodes".
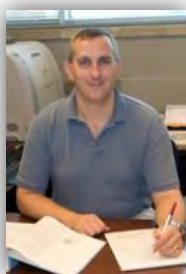
Dr. Steven Gwaltney was awarded a U.S. Department of Defense award for his project titled, "Molecular Modeling to Develop Better Reactivators".
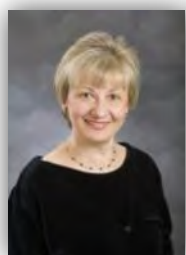
Dr. Ioana Banicescu and Dr. Sherif Abdelwahed received a grant by the Industry/University Cooperative Research Centers program of the National Science Foundation, Center for Autonomic Computing members from industry and government, and university matching funds to establish a Center for Autonomic Computing at Mississippi State University. Dr. Ioana Banicescu was honored with an invitation from the European Research Council to serve on the European Research Council Advanced Grant Evaluation Panel. This panel will be active from 2008-2013. The European Research Council promotes outstanding, frontier research in the sciences and humanities across Europe. Having a faculty member serve on this elite panel of this prestigious council is a superb achievement for MSU.

Dr. Hyeona Lim, Dr. Ratnasingham Shivaji, Dr. Xingzhou Yang, and Dr. Haimeng Zhang received a National Science Foundation Grant to host a Research Experience for Undergraduates (REU) site in Applied Mathematics and Bio-Statistics during the summers of 2010 and 2011. Also Dr. Lim and Dr. Shivaji received a National Science Foundation grant to host the 8th MSU-UAB Conference on Differential Equations and Computational Simulations.

CCS Funded Proposals since 2006

| Sponsor	Project Title	Amount	Personnel	Status
US Department of Army	Molecular Packing Software for Ad-Initio Crystal Structure	$17,474	Kim	Awarded (03/24/03 - 12/31/06)
ABSL Power Solutions, Inc.	Portable Energy Divisions: Composites, Modeling, and Integration, Task 2	$209,990	Novotny	Awarded (04/11/06 - 04/10/07)
Rensselaer Polytechnic Institute	Non Equilibrium Growth Phenomena and Scalability in Synchronized Computing Networks	$274,970	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	Lim, Shivaji	Awarded (08/15/07 - 07/31/08)
DOE	Nuclei at Extreme Conditions: A Relativistic Study (Awarded to Physics with overhead split to CCS)	$212,000	Afanasjevs	Awarded (12/15/06 - 11/14/09)
DOE	Nuclei at Extreme Conditions: A Relativistic Study	$222,000	Afanasjevs	Awarded (11/15/09 - 11/14/12)
Environment Canada	Changepoint Estimation for Canadian Sky-Cloudiness Frequencies Using a Temporal Continuation-Ratio Logit Model	$20,000	Lu	Awarded (12/01/08 - 03/31/09)
US Department of Defense	Molecular Modeling to Develop Better Reactivators (Ran through Center for Environmental Health Sciences (CEHS) with Overhead split between CCS and CEHS)	$48,900	Gwaltney	Awarded (01/11/07 - 01/10/10)
National Science Foundation	Collaborative Research : The role of isolation in species diversification: insights into dispersal and evolution of endemics Lotus	$99,777	Wallace	Awarded (03/01/09 - 02/29/12)
ERDC	Topological Features and Dynamics of Gene Flow Networks	$110,000	Brooks	Awarded (03/02/09 - 9/30/11)
MAFES/MS Soybean Promotion Board	Development of a Rapid Genetic Field Race Test for Soybean Cyst Nematode (SCN) and Generation of SCN Resistance through Gene Inactivation	$54,850	Klink, Lawrence, Koger, Allen, Balbalian	Awarded (04/01/09 - 3/31/10)
National Science Foundation	The Eighth Mississippi State- UAB Conference on Differential Equations and Computational Simulations	$35,000	Lim, Shivaji	Awarded (06/15/09 - 5/31/10)
National Science Foundation	Planning of a Center for Autonomic Computing	$10,000	Banicescu, Abdelwahed	Awarded (07/01/09 - 6/30/10)
DOE	Theory of Coexisting Density Waves in Low Dimensional Quarter-Filled Band Molecular Solids	$540,282	Clay	Awarded (09/01/08 - 8/31/12)

National Science Foundation	REU site Project: REU in Applied Mathematics and Biostatistics	$200,000	Lim. Shivaji, Yang, Zhang	Awarded (09/15/09 - 08/31/11)
MS Soybean Promotion Board	Identifying Full-Length Open Reading Frames of Genes involved in Interactions between Soybean and Nematodes	$35,000	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	Yang	Awarded (01/01/10 - 12/31/10)
ORED (Mississippi State University) (RIP)	Estimation of Latent Class Models with Conditional Dependence Using Multivariant Probit Analysis	$10,000	Xu	Awarded (01/01/10 - 12/31/10)
National Science Foundation	Characterization of cpDNA SSR's in Lotus for inferring phylogeographic patterns on the Channel Islands	$7000	Wallace	Awarded 2009 – 2012
Army Research Laboratory	Tailoring Magnetic Properties of Hexagonal Ferrites for Army Application	$15,000	Kim	Awarded 2010 - 2011
ORED (Mississippi State University)	Magnetic Materials properties (*MMN)* Research Group	$2000 (ORED)	Kim, Novotny, Clay, Koshka Gwaltney Singh, Shivaji Lim	Awarded 2010 – 2011
National Science Foundation Award	Differential Equations Weekend Seminar Awarded to University of Memphis with Shivaji serving as Co-PI	$14,500	Shivaji, G Goldstine (Uni. Of Memphis), J. Goldstine (Uni. Of Memphis)	Awarded 2008-2013
Indo-US Science and Technology Forum	Integrated study of correlated electrons in organic and inorganic materials	$55,000	Torsten Clay	Awarded 10/07 – 02/11
National Science Foundation And Industry	Center for Autonomic Computing at Mississippi State University	$1,259,937	Banicescu, Abdelwahed	Awarded (08/01/10– 07/31/15)

CCS Pending Proposals

Sponsor	Project Title	Amount	Personnel	Status
Federal Initiative for Funding (2010-2011) Department of Defense	**Advanced Materials Design for Nano Devices**	**$7.02M**	**Clay, Gwaltney, Kim, Lim, Novotny, Ray, Shivaji, Singh, Hong**	**Pendi ng**
Federal Initiative for Funding (2011-2012) Department of Defense	**Advanced Materials Design for Nano Devices**	**$8,200,384**	**Kim, Novotny Clay, Koshka S. Gwaltney, Singh, Shivaji Lim, Hong**	**Pending**
National Science Foundation (Limited Submission Proposal)	**Voltage-switching non-volatile magnetoelectric random access memory (MERAM) cells operating at room temperature based on multiferroic hexaferrites**	**$1,502,099**	**Kim, Novotny, Koshka, Hong**	**Pending**
Federal Initiative for Funding (2010-2011) Department of Defense	Towards Reliable and Green Computing Systems: An Automatic Management Approach	$2,599,651	Banicescu, Abdelwahed	Pending
National Science Foundation	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	Klink	Pending
National Science Foundation	Materials Inspired by Network Theory	$488,960	Novotny	Pending
National Science Foundation	Assessmant of Continental-Level Global Iindustrial-age Anthropogenic Inputs of Heavy Metals and Trace Elements in the Pedosphere	$1,257,051	Qi Qi Lu	Pending
Nuclear Energy University Programs	Multiscale Modeling of Creep Deformation in Nuclear Structural Materials	-	Novotny	Pending
National Science Foundation	Accelerating Technology Translation for Parallel Discrete Event Simulations	-	Novotny	Pending

Other Recent Proposals

Sponsor	Project Title	Personnel
Ultralife Corporation	Confirmation and Development of a Fast-Charging Method for Lion-Cells	Novotny, Wipf
NSF	CDI-Type II; Perfectly Scalable Asynchronous Computing: Theory, Algorithms, and Implementations	Novotny, Kim, Banicescu
DHS/SERRI	Developing A Quantitative Risk Model for Ranking Alternative Transportation Security Measures	Jin, Lu, Ling
NASA	Enhancing the Wildland Fire Assessment System using NASA Assets, Models, and Resources	Cooke, Anantharaj, Choi, Lu, Dixon, Jolly
SERRI	Developing A Quantitative Risk Model for Ranking Alternative Transportation Security Measures	Zhang, Lu, Jin, Ling
NSF	4D CFD; A Spatiotemporal Approach to Fluid Dynamics	Walters, Banicescu,green
DOE	Integrated Simulations and Experiments to Develop Reforming Catalyst for Renewable Hydrogen Production from Glycerin	Gwaltney, Kim, Kim, Fernando
NSF	Ecological Influences on the Evolutionary Diversification of Orchids: A Multidisciplinary Study of Landscape Genetics, Floral Morphology and Selection in Plantanthera Dilatata	Wallace
NSF (EPSCoR)	Modeling of Microsatellites in Generating Evolutionary Potential	Welch
EPSCoR	Mississippi Consortium for Evolutionary Ecology Cyberinformatics	Ervin, Wallace, Brooks, Welch
EPSCoR	NSF EPSCoR Track II White Paper	Kim, Shivaji, Banisescu, Clay, Gwaltney, Lim, Novotny, Wallace, Brooks
EPSCoR	Multiscale Atomistic Modeling of biomolecules and polymers	Kim, Shivaji, Banisescu, Clay, Gwaltney, Lim, Novotny
NSF	CSUMS: Undergraduate Research and Training in Differential Equations and their Applications	Kim, Lim, Janus, Shivaji, Park
NSF	Major research Instrumentation (jointly with LSBI, IDB, and CCS)	Burgess, Banicescu, Bridges, Lawrence, Peterson
NSF	Efficient Numerical Methods for Variational Image Restoration and Segmentation	Lim
NSF	Composition Markov Chains of Multinomial Type	Zhang
NSF	A Mechanical and Computational Model of the Unicellular Green Algae Chlamydomonas	Yang
NSF	UBM Group: The Landscape Genetics of Plant-Pollinator Interactions – Integrating Models and Data	Brooks, Zhang, Wallace, Xu, Yuan
NSF	EMSW21-RTG Research Training in Partial Differential Equations with applications in Biology and Material Science	Lim, Shivaji, Yang, Yarahmadian
NSF	Tailoring Magnetic Properties of Hexagonal Ferrites	Kim
US DOE	Few-and Many-Body Nuclear Theory from QCD	Rupak
DOE	Universality, Nuclear Physics and QCD	Rupak
NSF	Collaborative Research: Magnolia grandiFLORA: A digital Herbarium of Collections in Mississippi	L. Wallace, C. Brooks, G. Ervin
NIH	Early Detection of Myocardial Infraction: A 3D Diffusion Tensor MRI Study on Heart Fiber Architecture	Zhang
NSF	Integrated Computational Materials Engineering (ICME) for Development of New Magnesium Alloys	Novotny

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