

**Mississippi State University**

**Center for Computational Sciences**

**2011 Annual Report**



## 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 crosscutting tools that allows a comprehensive, multi-disciplinary approach to problem solving.*

*Year 2011 major activities/initiatives include: (1) Research Experiences for Undergraduates (REU) Site in Applied Mathematics and Biostatistics; (2) a Center for Autonomic Computing; (3) Modeling Materials for Sustainable Energy; (4) An NSF funded project on high-T<sub>c</sub> superconductivity phenomena in layered organic and inorganic materials; (5) DOE funded project on rare-earth-free nanostructure permanent magnets; (6) Image processing in bio-inspired materials design; and (7) Hosting of the Southeastern Theoretical Chemistry Association (SETCA) 2011 annual meeting. Major events/proposals already planned in the near future include: (a) Ninth Mississippi State—Univ. of Alabama at Birmingham Conference on Differential Equations and Computational Simulations; and (b) An NSF Proposal for Integrative Graduate Education and Research Traineeship (IGERT) program Cyberinfrastructure (CIF21)-track.*

*This report will provide synopsis of these activities/initiatives, the list of CCS Personnel, the recent awards and recognitions, and research publications. Also included in the report are the details on funding activity. Overall, 2011 has been a successful year for CCS. We look forward to building on this platform, to achieve greater excellence in coming years.*



A handwritten signature in black ink that reads "Seong-Gon Kim".

Seong-Gon Kim  
Director, Center for Computational Sciences  
Associate Professor  
Department of Physics and Astronomy  
Mississippi State University

## *CCS Personnel*

**Director: Seong-Gon Kim, Associate Professor, Physics and Astronomy**

**Associate Director: Hyeona Lim, Associate Professor, Mathematics**

### **Biological Sciences**

**Christopher Brooks, Assistant Professor**

**Vincent Klink, Assistant Professor**

**Lisa Wallace, Assistant Professor**

### **Chemistry**

**Steven Gwaltney, Associate Professor**

### **Computer Science**

**Ioana Banicescu, Professor**

**Changhe Yuan, Assistant Professor**

**Song Zhang, Assistant Professor**

### **Electrical & Computer Engineering**

**Sherif Abdelwahed, Assistant Professor**

**Yaroslav Koshka, Associate Professor**

### **Industrial Engineering**

**Mingzhou Jin, Associate Professor**

### **Mathematics**

**Seongjai Kim, Associate Professor**

**Hyeona Lim, Associate Professor**

**Xingzhou Yang, Assistant Professor**

**Shantia Yarahmadian, Assistant Professor**

### **Physics**

**Anatoli Afanasjev, Professor**

**Matthew J. Berg, Assistant Professor**

**Torsten Clay, Associate Professor**

**Dipankar Dutta, Assistant Professor**

**Seong-Gon Kim, Associate Professor**

**Mark Novotny, Professor and Department Head**

**Gautam Rupak, Assistant Professor**

**Jinwu Ye, Associate Professor**

### **Statistics**

**Mohammed Sepehrifar, Assistant Professor**

**Jonathan Woody, Assistant Professor**

**Haimeng Zhang, Associate Professor**

### **College of Veterinary Medicine, Basic Sciences**

**Henry X.-F. Wan, Assistant Professor**

### ***CCS Proposal Submissions***

Fiscal Year	Total Amount	Number of Proposals
FY09	\$3,658,734	12
FY10	\$5,150,061	9
FY11	\$2,403,312	6
FY12	\$4,647,396	15

### ***CCS Awards***

Fiscal Year	Total Amount	Number of Awards
FY09	\$374,279	5
FY10	\$456,850	8
FY11	\$404,754	6
FY12	\$388,491	7

### ***CCS Research Expenditures***

Fiscal Year	Total Amount
FY09	\$303,807
FY10	\$442,078
FY11	\$565,413
FY12	\$573,625

## CCS Major Initiatives

### Research Experiences for Undergraduates (REU) Site in Applied Mathematics and Biostatistics

Dr. Hyeona Lim is the PI for the NSF funded Research Experiences for Undergraduates (REU) Program in Applied Mathematics and Biostatistics (NSF-0852032, September, 2009 - August, 2012, Award amount: \$200,000) which was hosted by the CCS and the Department of Mathematics and Statistics. This REU site program is aimed to provide the participants

with meaningful research experiences, to show them the enjoyment of doing research, and to encourage them to pursue advanced degrees in mathematical sciences. For the last two years (2010 & 2011), 12 highly talented undergraduate students (mostly from outside institutions) were selected among 151 applicants. These students spent their summers on MSU campus and successfully finished research projects under the supervision of 4 faculty members in Mathematics and Biostatistics (Drs. Hyeona Lim, Ratnasingham Shivaji, Haimeng Zhang, and Xingzhou Yang). Two of the 2010 REU students were admitted to the graduate program in mathematics at Mississippi State University (MSU) in Fall 2011. The REU students participated in 6 different conferences and gave 18 oral presentations on their projects. The participants also gave poster presentations at the Undergraduate Research Symposium, hosted by Shackouls Honors College at MSU in 2010 & 2011. One of the students won the 1<sup>st</sup> place award for his poster presentation among over 50 posters at the Symposium. Several papers were submitted or are planning to be submitted to academic journals. In order to disseminate new findings from our REU program, a one-day Research Experiences for Teachers (RET) workshop was organized on February 4, 2012 for Mississippi and a few other states' high school teachers in mathematical sciences.



**RESEARCH EXPERIENCES FOR UNDERGRADUATES**  
in APPLIED MATHEMATICS & BIostatISTICS  
MAY 30 - AUGUST 7, 2010  
MISSISSIPPI STATE UNIVERSITY  
WWW.MSSTATE.EDU/DEPT/MATH/EVENTS/REU

**Summary**  
\$4,500 Stipend and \$750 Travel Allowance  
Free On-campus Housing and Allowance for Meals  
Variety of Research Opportunities  
Experienced Faculty Mentoring  
Weekend Social Activities

**Eligibility**  
US Citizens or Permanent Residents  
Background in Multivariable Calculus, Linear Algebra, and Ordinary Differential Equations or Probability  
Women and students from underrepresented groups are particularly encouraged to apply

**APPLICATION DEADLINE: FEBRUARY 15, 2010**  
**ONLINE APPLICATION:**  
**WWW.MSSTATE.EDU/DEPT/MATH/EVENTS/REU**

For more information contact:  
Hyeona Lim, R. Shivaji, Xingzhou Yang, or Haimeng Zhang at [reu@math.msstate.edu](mailto:reu@math.msstate.edu)

MISSISSIPPI STATE UNIVERSITY Arts & Sciences CCS HPC<sup>2</sup>



**RESEARCH EXPERIENCES FOR UNDERGRADUATES**  
in APPLIED MATHEMATICS & BIostatISTICS  
MAY 31 - AUGUST 6, 2011  
MISSISSIPPI STATE UNIVERSITY

**Summary**  
\$4,500 Stipend and \$750 Travel Allowance  
Free On-campus Housing and Allowance for Meals  
Variety of Research Opportunities  
Experienced Faculty Mentoring  
Weekend Social Activities

**Eligibility**  
US Citizens or Permanent Residents  
Background in Multivariable Calculus, Linear Algebra, and Ordinary Differential Equations or Probability  
Women and students from underrepresented groups are particularly encouraged to apply

**APPLICATION DEADLINE: FEBRUARY 15, 2011**  
**ONLINE APPLICATION:**  
**WWW.MSSTATE.EDU/DEPT/MATH/EVENTS/REU**

For more information contact:  
Hyeona Lim, R. Shivaji, Xingzhou Yang, or  
Haimeng Zhang at [reu@math.msstate.edu](mailto:reu@math.msstate.edu)

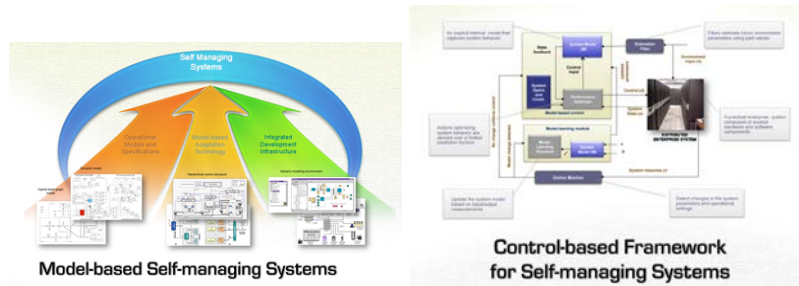
MISSISSIPPI STATE UNIVERSITY Arts & Sciences CCS HPC<sup>2</sup>

## ***Center for Autonomic Computing:***

CCS is pleased to announce that the NSF Center for Autonomic Computing (NSF CAC) at MSU led by Dr. Ioana Banicescu and Dr. Sherif Abdelwahed successfully continued its research activities during the second year. The NSF CAC was initiated as a consortium of four universities: University of Florida, University of Arizona, Rutgers University, and Mississippi State University, and it is funded by the NSF I/UCRC program of the National Science Foundation, CAC members from industry, government laboratories, and university matching funds. The goals of the center are: 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; and to accelerate the creation and transfer of knowledge and technology for autonomic computing into industry and commercial products. The technical scope of the center focuses on autonomic computing (AC) systems. These systems use self-management techniques to enable independent and efficient operation, minimize cost and risk, accommodate various complexities and uncertainties of the environment, or command systems with large numbers of components.

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. A number of proposals for continuing support of the center have been submitted to NSF, and the Fundamental Research Program (FRP) funded the proposal: "Collaborative Research: Towards Unified Cloud Computing and Management". 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 and MSU State Pride Awards. In October 2011, Dr. Ioana Banicescu was a keynote speaker at the International Conference on System Theory Control and Computing (IS-CTCC2011).

For additional information, visit the NSF CAC at MSU page at <http://www.nsfcac.msstate.edu>

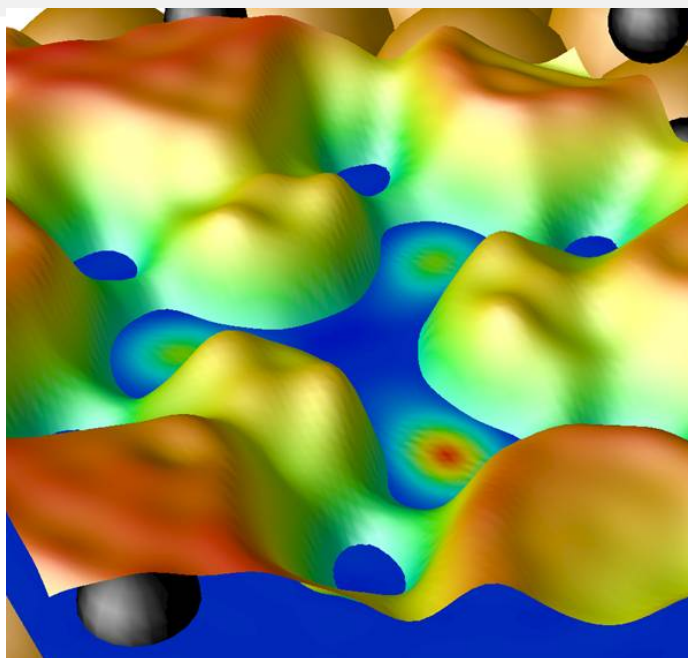




## Modeling Materials for Sustainable Energy

Dr. Seong-Gon Kim is leading a team of 20 faculty to submit a proposal (\$3.5 million) to the NSF IGERT-CIF21 Program to develop new materials for sustainable energy

Sustainable energy – energy that is *accessible, clean* and *efficient* – is critical in solving the global energy problem. According to United Nations nearly one in five people around the world do not have access to modern energy services while twice that number, three billion people, rely on wood, coal, charcoal, or animal waste for cooking and heating, creating a major barrier to eradicating poverty. A UN-led global initiative on Sustainable Energy for All is calling for action from all

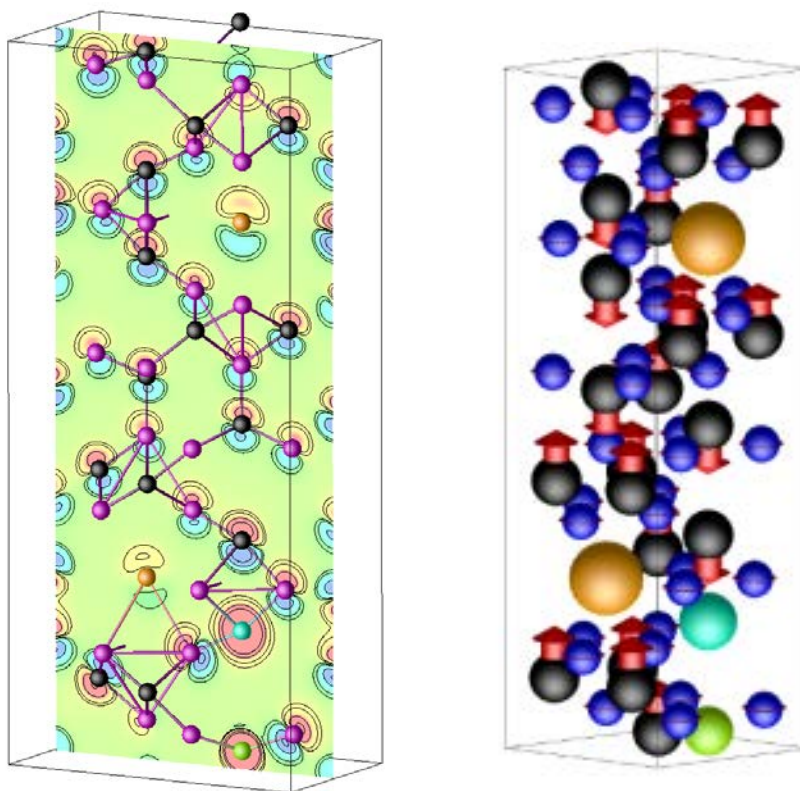


sectors of society in support of three interlinked objectives to be achieved by 2030: providing universal access to modern energy services; doubling the global rate of improvement in energy efficiency; and doubling the share of renewable energy in the global energy mix. These critical objectives can only be met when we have the required technology. Materials play a key role in enabling technologies that can offer promising solutions to achieve renewable and sustainable energy pathways, leading to sustained prosperity for all human kind. With our proposed IGERT-CIF21 program, we will train future materials scientists and engineers with the necessary knowledge and experiences to be ready to tackle the challenge of providing sustainable energy for all. The *goal* of this IGERT program is to support and train at least 25 graduate students at Mississippi State University in interdisciplinary research in Materials for Sustainable Energy as they pursue their respective PhD programs. Over the next five years the project will focus on three major research themes: fundamentals of materials, the application of new materials to sustainable energy technologies, and the development of cyberinfrastructure necessary to facilitate this research. This program will bring together graduate students across the campus and from regional universities with a unified research theme. Students who participate in our IGERT program will be well-trained and able to step into leadership positions in their fields. Support for industrial and federal internships and for international travel and research will ensure a well-rounded education.



## Rare-earth-free nanostructure permanent magnets

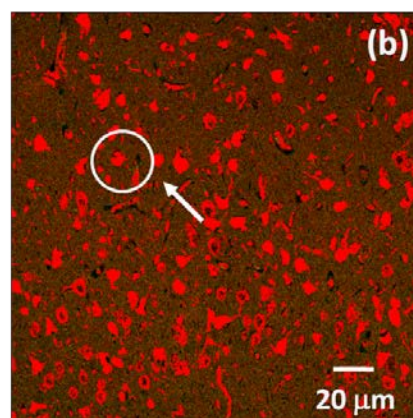
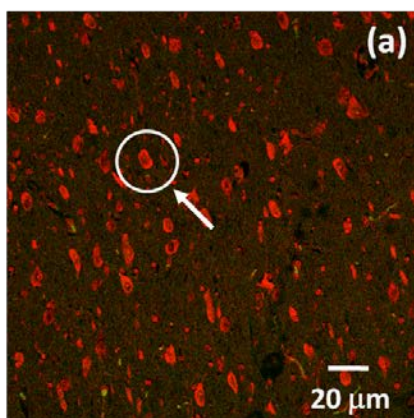
Dr. Seong-Gon Kim is leading a Department of Energy (DOE) funded research project to develop new materials for rare-earth (RE)-free permanent magnets for sustainable energy applications. Rare earths are naturally occurring minerals with unique magnetic properties that are used in electric vehicle (EV) motors and wind generators. Because these minerals are expensive and in limited supply, improvements must be made to encourage existing technologies to use rare earths more efficiently, or to replace them altogether with inexpensive and abundant



materials like nickel and manganese. Alternatives to rare earths will contribute to the cost-effectiveness of EVs and wind generators, facilitating their widespread use and drastically reducing the amount of greenhouse gases released into the atmosphere. Dr. Kim's team is developing new Sr/Ba-hexaferrite-based materials doped with various non-RE elements for use in the electric motors of EVs and renewable power generators that will demonstrate magnetic properties superior to today's best rare earth magnets. EVs and renewable power generators typically use rare earths to make their electric motors smaller and more powerful. However, RE's are difficult to locate, time-consuming to extract and expensive to refine. This research has the potential to improve upon the performance of current state-of-the-art rare earth magnets using low-cost and more abundant materials such as manganese and iron.

### Image Processing in Bio-inspired Materials Design (IPBMD)

Dr. Hyeona Lim is a PI of this cross college research grant sponsored by



the ORED at MSU. This is an interdisciplinary effort with bio-inspired materials design team at CAVS. Co-PIs are Drs. Yuxiong (Max) Mao, Raj Prabhu, Lakiesha Williams, Jun Liao, Hongjoo Rhee, Mark Horstemeyer, and Ricolindo Carino. Bio-inspired materials design of the protective gears (*e.g.*, helmet, body armor, etc.) is at the forefront of state-of-the-art research. Unlocking the hierarchical design also involves a detailed study of the materiality (microstructural feature) and morphometry in diverse mechanical loads. However, image processing and analysis in bio-inspired materials design is in a nascent stage; especially, in capturing the physics of the hierarchical-based design of biomaterials. For instance, when the brain parenchyma is imposed to mechanical loads that cause Traumatic Brain Injury (TBI), the neuron cells incur biological damage (Figure 1) and subsequent death. Quantification of the biological damage is possible through observation of the change in the geometry of the neuron cells. This structure-property correlation is pivotal to understanding the mechanism of damage. Such information could be used to design better protective gears.

### **Cross-disciplinary Undergraduate Research and Education (CURE)**

Dr. Hyeona Lim is the PI of this cross college research grant sponsored by the ORED at MSU. Co-PIs are Drs. Andy Perkins, Erdogan Memili, Jenny Du, Chris Brooks, Matthew Berg, Donna Pierce, Seong-Gon Kim, Hongjoo Rhee, Wendy Herd, Sandra Eksioglu, and Burak Eksioglu. The objectives are to form a team of researchers in the areas of Science, Technology, Engineering, and Mathematics (STEM) at MSU interested in conducting research with undergraduate students and to discuss/share ideas on undergraduate research and education, promote collaborative efforts among members of the CURE Group through regular meetings, and seek external grant application to the National Science Foundation (NSF) Programs such as interdisciplinary Research Experiences for Undergraduates (REU), Transforming Undergraduate Education in STEM (TUES), Computational Science Training for Undergraduates in the Mathematical Sciences (CSUMS), etc., and to recruit more undergraduate students in the STEM area at MSU. All of the CURE Group members are experienced researchers and dedicated mentors. Three of the group members are involved in the NSF-funded undergraduate research programs. Hyeona Lim is the PI for the NSF-REU in Applied Mathematics and Biostatistics (NSF-0852032, September, 2009 - August, 2012, Award amount: \$200,000) which was hosted by the CCS and the Department of Mathematics and Statistics. Andy Perkins is the PI for the NSF-funded REU in Computational Biology, hosted by the Computer Science and Engineering Department. This REU has involved 11 faculty mentors from Computer Science and Engineering, Biochemistry and Molecular Biology, Animal and Dairy Sciences, CVM Basic Sciences, and Biological Sciences. Erdogan Memili is the PI for the NSF funded Undergraduate Research and Mentoring (URM) in Functional Genomics, hosted by the Department of Animal and Dairy Sciences in 2010 & 2011.

## The 9th Mississippi State-UAB Conference on Differential Equations and Computational Simulations

The 9th Mississippi State-UAB Conference on Differential Equations and Computational Simulations will be held on October 4-6, 2012 in McCool Hall, at MSU. Dr. Hyeona Lim has recently obtained the NSF grant of \$35,000 to support travel expenses of graduate students and recent Ph.D.s. The conference website is <http://www.ccs.msstate.edu/deconf/de2012/>. Mississippi State-UAB conference series on Differential Equations and Computational Simulations has hosted eight highly successful conferences since 1993. More information on the past eight conferences can be found at [http://www.ccs.msstate.edu/deconf/de2012/PastDE\\_Confs\\_Brochure.pdf](http://www.ccs.msstate.edu/deconf/de2012/PastDE_Confs_Brochure.pdf). Dr. Ratnasingham Shivaji from MSU and Dr. Bharat Soni from University of Alabama at Birmingham (UAB) served as organizers for these international conferences. The ninth conference of the series will be hosted by the CCS and the Department of Mathematics and Statistics at MSU, and the Department of Mechanical Engineering at UAB. Dr. Hyeona Lim and Dr. Roy Koomullil (UAB) will serve as new organizers of this conference series. 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. In addition to the ten principal lectures, there will be sessions for twenty minute contributed talks. This conference will also be dedicated to Alfonso Castro in celebration of his 62nd birthday and his outstanding contributions to differential equations. Conference participants are encouraged to submit full length manuscripts after the conference. Reviewed manuscripts will be published as a special issue of the Electronic Journal of Differential Equations. Pre-registration deadline is August 31, 2012. Abstracts for contributed papers should be submitted electronically no later than August 31, 2012. Contributed papers will be included in the final program only if pre-registration is complete. For further information regarding the organization, program, and submission of abstracts, visit the conference website at <http://www.ccs.msstate.edu/deconf/de2012> or contact the program chair Jerome Goddard II (Auburn University Montgomery) at [decs@math.msstate.edu](mailto:decs@math.msstate.edu), or the organizers:

Mississippi State - UAB Conference on  
**9th DIFFERENTIAL EQUATIONS & COMPUTATIONAL SIMULATIONS**  
October 4-6, 2012  
McCool Hall  
Mississippi State University

**Principal Speakers:**

MONICA CLAPP, Universidad Nacional Autónoma de México, Mexico	MYTHILY RAMASWAMY, Tata Institute of Fundamental Research, India
DAVID A. DIXON, University of Alabama	CHI-WANG SHU, Brown University
STEVE ROBINSON, Wake Forest University	EITAN TADMOR, University of Maryland
DEAN SICKING, University of Nebraska-Lincoln	JORGE VINALS, University of Minnesota
PETER TAKAC, Universität Rostock, Germany	ZHI WANG, Iowa State University

This interdisciplinary conference will provide a joint forum where mathematicians, scientists and engineers from industries, federal laboratories and academia can exchange research and development ideas. An overall goal of this conference is to promote research and education in mathematical and computational analysis of theoretical and applied differential equations. In addition to the ten principal lectures, there will be sessions for twenty minute contributed talks. This conference will also be dedicated to Alfonso Castro in celebration of his 62nd birthday and his outstanding contributions to differential equations. Conference participants are encouraged to submit full length manuscripts after the conference. Reviewed manuscripts will be published as a special issue of the Electronic Journal of Differential Equations. Pre-registration deadline is August 31, 2012. Abstracts for contributed papers should be submitted electronically no later than August 31, 2012. Contributed papers will be included in the final program only if pre-registration is complete. For further information regarding the organization, program, and submission of abstracts, visit the conference website at <http://www.ccs.msstate.edu/deconf/de2012> or contact the program chair Jerome Goddard II (Auburn University Montgomery) at [decs@math.msstate.edu](mailto:decs@math.msstate.edu), or the organizers:

Hyeona Lim • Associate Professor of Mathematics  
Associate Director, Center for Computational Sciences  
Dept. of Mathematics & Statistics  
Center for Computational Sciences  
Mississippi State University

Roy Koomullil • Associate Professor  
Dept. of Mechanical Engineering  
University of Alabama Birmingham

UAB MISSISSIPPI STATE UNIVERSITY

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

### Plant Conservation Genetics Workshop:

As part of a current NSF-funded project studying phylogeographic patterns of plants on the California Channel Islands, Dr. Lisa Wallace co-hosted a workshop with Dr. Mitchell McGlaughlin of the University of Northern Colorado and Dr. Kaius Helenurm of the University of South Dakota entitled *Plant Conservation Genetics*. The workshop was held January 10-11, 2012 at the Town and Country Resort in San Diego, CA and in conjunction with the annual meeting of the California Native Plant Society. They were able to provide travel grants from the NSF funds to most of the attendees, who included graduate students and conservation biologists with the National Park Service, U.S. Navy, Santa Catalina Island Conservancy, U.S. Fish and Wildlife Service, Bureau of Land Management, and several botanical gardens throughout

the U.S. During the workshop, they provided information on the collection and interpretation of genetic data as they relate to the conservation of rare plants.

## **Southeastern Theoretical Chemistry Association 2011 Annual Meeting at MSU**

Dr. Steven Gwaltney co-hosted the Southeastern Theoretical Chemistry Association (SETCA) 2011 annual meeting at MSU. The SETCA 2011 annual meeting brought eighty theoretical and computational chemists from around the Southeast to MSU for a two day conference. The program included 9 invited lectures and 6 contributed lectures, in addition to 29 poster presentations. The 2011 conference was the 42nd year for the annual meeting and was the first time the meeting has been held at MSU. Hosting the conference served to highlight the role of computational science and CCS at MSU and provided a chance to "show off" our facilities and capabilities to leaders in the field in this region of the country.

## ***CCS Current Funded Projects***

1. R.T. Clay, Indo-US Science and Technology Forum, "Integrated study of correlated electrons in organic and inorganic materials," , \$55,000, Awarded 2007-2011
2. C. Brooks, ERDC, Topological Features and Dynamics of Gene Flow Networks, \$110,000, Awarded, 2009-2011
3. Seong-Gon Kim, Army Research Laboratory , Tailoring Magnetic Properties of Hexagonal Ferrites for Army Application , \$15,000, Awarded, 2010 - 2011
4. Kim, Novotny, Clay, Koshka, Gwaltney , ORED (Mississippi State University), Magnetic Materials properties (MMN) Research Group, \$2000 (ORED), Awarded, 2010 –2011
5. L.E. Wallace , Graduate Assistant Bridge Funds, Graduate Assistant Bridge Funds, \$17,500, Greg Wheeler, Awarded, 2011
6. S.Abdelwahed, ONR, Advanced Naval Power Systems through Electric Ship Systems Research and Development, \$269,669, Awarded, 2008 - 2011
7. Lim. Shivaji, Yang, Zhang, National Science Foundation, REU site Project: REU in Applied Mathematics and Biostatistics, \$200,000, Awarded, 2009-2012
8. S.Abdelwahed, National Science Foundation, Towards Unified Cloud Computing and Management, \$50,000, Awarded, 2011- 2012
9. R.T. Clay, US Department of Energy (DOE-Basic Energy Sciences), Charge frustration, spin singlets and superconductivity in the 1/4-filled band paired-electron crystal, \$420,000, Awarded, 2009-2012
10. Afanasjevs, DOE, Nuclei at Extreme Conditions: A Relativistic Study, \$222,000, Awarded, 2009-2012
11. S.Abdelwahed, ONR, Advanced Naval Power Systems through Electric Ship Systems Research and Development - Continuation, \$300,000, Awarded, 2012 – 2012
12. L.E. Wallace, The Mohamed bin Zayed Species Conservation Fund, Development of microsatellite markers in Caribbean iguanas, \$10,000, M.E. Welch, et al, Awarded, 2012
13. H. Lim, A. Perkins, E. Memili, J. Du, C. Brooks, M. Berg, D. Pierce, S-G Kim, H. Rhee, ORED, Mississippi State University, Cross College Research Program, Cross-disciplinary Undergraduate Research and Education (CURE) Group, \$2,000, Awarded, 2011-2012
14. H. Lim, Y. Mao, R. Prabhu, L. Williams, J. Liao, H. Rhee, M. Horstemeyer, ORED, Mississippi State University, Cross College Research Program, Image Processing in Bio-inspired Materials Design (IPBMD) Group, \$2,000, Awarded, 2011-2012
15. R. T. Clay, DOE, Theory of Coexisting Density Waves in Low Dimensional Quarter-Filled Band Molecular Solids, \$540,282, Awarded, 2008-2012
16. I. Banicescu, S. Abdelwahed, National Science Foundation, Collaborative Research: Towards Unified Cloud Computing and Management, \$50,000, Awarded, 2011- 2012
17. L. Wallace, National Science Foundation, Characterization of cpDNA SSR's in Lotus for inferring phylogeographic patterns on the Channel Islands, \$7000, Awarded, 2009 –2012
18. Ioana Banicescu, Shane Burgess, Bindu Nanduri, Daniel Peterson, National Science Foundation (MRI), Acquisition of Integrated Infrastructure Enabling Multidisciplinary Research in System Biology, \$800,867, Awarded, 2009-2012

19. H. Lim, Shivaji, Institute for Mathematics and its applications, The 9<sup>th</sup> Mississippi State-UAB Conference on Differential Equations and Computational Simulations, \$5,000, Awarded, 2011-2012
20. Klink, MS Soybean Promotion Board, Identifying Full-Length Open Reading Frames of Genes involved in Interactions between Soybean and Nematodes, \$35,000, Awarded, 2009-2013
21. Shivaji, G Goldstine (Uni. Of Memphis), J. Goldstine (Uni. Of Memphis), National Science Foundation Award, Differential Equations Weekend Seminar, \$14,500, Awarded, 2008-2013
22. L.E. Wallace, K. Helenurm and M.E. McGlaughlin, National Science Foundation, Collaborative Research: The role of isolation in species diversification; insights into dispersal and evolution of endemic Lotus from the California Channel Islands, \$99,777 at MSU Three REU Supplements, \$7,000(2010); \$7,492(2011); \$7,500 (2012), Awarded, 2009-2013
23. Hyeona Lim, National Science Foundation , The 9<sup>th</sup> Mississippi State –UAB Conference on Differential Equations and Computational Simulations, \$35,000, Awarded, 2012-2013
24. I. Banicescu, S. Abdelwahed, National Science Foundation And Industry, Center for Autonomic Computing at Mississippi State University, \$1,259,937, Awarded, 2010-2015
25. R. T. Clay, US Department of Energy (DOE-Basic Energy Sciences), Theory of layered organic and inorganic materials with charge spin frustration, \$636,000, Awarded, 2009-2015
26. S.Abdelwahed, National Science Foundation, Establishing a Center for Autonomic Computing at Mississippi State University, \$1,351,862, Awarded, 2010 –2015



## *Publications*

### *Patents*

M. Novotny, Patent No. 12/590,717 filed 11/12/2009, "System and Method for Charging Rechargeable Batteries".

### *Refereed Journals*

1. V. Afanasjev, H. Abusara, E. Litvinova, P. Ring, Spectroscopy of the heaviest nuclei (theory), *Journal of Physics: Conference Series* 312 (2011) 092004: 1-10
2. Classes of infinite semipositone  $n \times n$  systems, Eun Kyoung Lee, R. Shivaji and Jinglong Ye, *Differential Integral Equations*, Vol. 24, No. 3-4(2011) , pp. 361-370.
3. Banicescu and H. Lim and R. Carino and S. Kim, A parameter study of a hybrid Laplacian mean-curvature flow denoising model. *Journal of Supercomputing*, Vol. 57, No. 3, pp. 339–356 (2011).
4. H. Kim, Y. Cha, and S. Kim, Curvature interpolation method for image zooming. *IEEE Trans. Image Process.*, Vol. 20, No. 7, pp. 1895–1903 (2011).
5. Nonexistence results for classes of  $3 \times 3$  elliptic systems, R. Shivaji and Jinglong Ye, *J. Nonlinear Analysis, TMA*, Vol. 74 (2011), pp. 1485-1494.
6. Positive solutions for  $n \times n$  Laplacian systems with combined nonlinear effects, Jaffar Ali, K. J. Brown and R. Shivaji, *Differential Integral Equations*, Vol. 24, No. 3-4 (2011), pp. 307-324.
7. Sungho Kim, Seong-Gon Kim, Mark Horstemeyer, "Vanadium effects on a BCC iron sigma 3 grain boundary strength", *Proceedings: Collected Proceedings: Deformation, Damage, and Fracture of Light Metals and Alloys* (2011).
8. P. Ring, H. Abusara, A. V. Afanasjev, G. A. Lalazissis, T. Niksic, and D. Vretenar, Modern applications of covariant density functional theory *International Journal of Modern Physics E*, vol. 20, No. 2, (2011) 235-243
9. E. V. Litvinova and A. V. Afanasjev, Dynamics of nuclear single-particle structure in covariant theory of particle-vibration coupling: From light to superheavy nuclei *Physical Review C* 84 (2011) 014305: 1-19
10. Shantia Yarahmadian, Blake Barker, Sidney Shaw, and Kevin Zumbrun, Existence and Stability of Steady States of a Reaction Convection Diffusion Equation Modeling Microtubule Formation, *Journal of Mathematical Biology*, Accepted in 2010, will be published in Vol 62, Issue 1, 2011.
11. S. Nouranian, C. Jang, T. E. Lacy, S. R. Gwaltney, H. Toghiani, and C. U. Pittman, Jr., "Molecular dynamics simulations of vinyl ester resin monomer interactions with a vapor-grown carbon nanofiber and their implications for composite interphase formation," *Carbon* 49, 3219-3232 (2011)
12. T. E. Lacy, S. Gwaltney, C. U. Pittman, Jr., H. Toghiani, C. Jang, S. Nouranian, and J. Yu, "Some Key Issues in Multi-Scale Modeling of Thermoset Nanocomposites/Composites," in *Tools, Models, Databases, and Simulation Tools Developed and Needed to Realize the Vision of Integrated Computational Materials Engineering*, edited by S.M. Arnold and T. Wong (ASM International, Materials Park, OH, 2011) pp. 128-140.

13. C. Jang, S. Nouranian, T. E. Lacy, S. R. Gwaltney, H. Toghiani, and C. U. Pittman, Jr., "Molecular dynamics simulations of oxidized vapor-grown carbon nanofiber surface interactions with vinyl ester resin monomers," *Carbon* 50, 748-760 (2012) (DOI: 10.1016/j.carbon.2011.09.013).
14. H. Li, RTC, S. Mazumdar, "Theory of carrier concentration-dependent electronic behavior in layered cobaltates," *Physical Review Letters* 106, 216401 (4 pages) (2011)
15. S. Dayal, RTC, H. Li, S. Mazumdar, "Paired electron crystal: Order from frustration in the quarter-filled band," *Physical Review B* 83, 245106 (12 pages) (2011) (Selected as an "Editors' suggestions" paper)
16. Banicescu, H. Lim, R. Carino, and S.J. Kim. A Parameter Study of a Hybrid Laplacian Mean-Curvature Flow Denoising Model, *Journal of Supercomputing*, Vol. 57, pages 339-356, 2011. Banicescu, R. Carino, J.L Harvill, J. P. Lestrade. Investigating Asymptotic Properties of Vector Nonlinear Time Series Models", *Journal of Computational and Applied Mathematics*, Vol. 236, pages 411-421, 2011.
17. P.J. Vardon, P. Cleall, H. R. Thomas, R.N. Philp., I. Banicescu, Three-dimensional Field-scale Coupled Thermo-Hydro-Mechanical Modeling: Parallel Computing Implementation, *International Journal of Geomechanics*, Vol.11(2), pages 90-98, 2011.
18. Ying Dong, Jinwu Ye and Han Pu, Multi-stability in an optomechanical system with two-component Bose-Einstein condensate, *Phys. Rev. A* 83, 031608 (R) (2011).
19. Jinwu Ye, J.M. Zhang, W.M. Liu, K.Y. Zhang, Yan Li, W.P. Zhang, Light scattering detection of various quantum phases of ultracold atoms in optical lattices, *Phys. Rev. A* 83, 051604 (R) (2011).
20. Jinwu Ye and CunLin Zhang, Super-radiance, Berry phase, Photon phase diffusion and Number squeezed state in the  $U(1)$  Dicke ( Tavis-Cummings ) model *Phys. Rev. A* 84, 023840 (2011).
21. Y.-L. Pan, M. J. Berg, S. S.-M. Zhang, H. Noh, H. Cao, R. K. Chang, and G. Videen, "Measurement and autocorrelation analysis of two-dimensional light-scattering patterns from living cells for label-free classification," *Cytometry A* 79 p. 284-92 (2011).
22. M. J. Berg, "The cause of characteristic lengths in scattering curves," *Atti della Accademia Peloritana dei Pericolanti* 89 p. C1V89S1P018 (2011).
23. M. J. Berg and G. Videen, "Digital holographic imaging of aerosol particles in flight," *J. Quant. Spectros. Radiat. Transfer* 112 p. (2011).
24. *J. Physics A: Mathematical and Theoretical* 44, 345004 [18 pages] (2011), with former PhD student Katja Biswas, "Mapping the Dynamics of Complex Multi-dimensional Systems into a Discrete Set of States Conserving the Mean-First-Passage Time: A Projective Dynamics Approach" *Physical Review E* 83, 041106 [12 pages], with former MS student Chris Varghese and S. Boettcher of Emory U, "Quantum Transport through Hierarchical Structures"
25. Shantia Yarahmadian, Blake Barker, Kevin Zumbrun, and Sidney L. Shaw, Existence And Stability Of Steady States Of A Convection Diffusion Equation Modeling Microtubules Formation, *Journal of Mathematical Biology* Volume 63, Issue 3 (2011), Page 459-492
26. M. J. Berg, C. M. Sorensen, A. Chakrabarti, "A new explanation of the extinction paradox," *J. Quant. Spectros. Radiat. Transfer* 112 p. 1170-81 (2011).

27. D. Dutta, J-C. Peng, I. C. Cloet and D. Gaskell, Pion-induced Drell-Yan processes and the flavor-dependent EMC effect," *Phys. Rev. C* 83, 042201R (2011).
28. Single spin asymmetries in charged pion production from semi-inclusive deep inelastic scattering on a transversely polarized  $^3\text{He}$  target," *Phys. Rev. Lett.* 107, 072003 (2011).
29. Nuruzzaman, D. Dutta et al., Nuclear transparency and effective kaon-nucleon cross section from the  $A(e,e'K^+)$  reaction," *Phys. Rev. C* 84, 015210 (2011).
30. D. Dutta, Feasibility of a spin-light polarimeter at JLab, *J. Phys. Conf. Ser.*, 295, 012141 (2011).
31. Search for effects beyond the Born approximation in polarization transfer observables in elastic scattering," *Phys. Rev. Lett.* 106, 132501 (2011).
32. Transverse momentum dependent parton distributions/fragmentation functions at an electron-ion collider," *Eur. Phys. J. A* 47, 35 (2011).
33. Rao, M.B., Kasala, S., and Zhang, H. Probabilistic recurrence relations, *Advances in directional and linear statistics. A Festschrift Volume for J S Rao*, Springer, chapter 15, pp 217 – 233. (2011)
34. Goldstein, L. and Zhang, H. "A Berry Esseen Bound for the Lightbulb Process". *Advances in Applied Probability*, Vol. 43, pp 875-898. (2011)
35. Changhe Yuan, Heejin Lim, Tsai-Ching Lu. Most Relevant Explanation in Bayesian Networks. *Journal of Artificial Intelligence Research (JAIR)*. Vol. 42. Pages 309-352. 2011.
36. Changhe Yuan, Heejin Lim, Michael L. Littman. Most Relevant Explanation: Computational Complexity and Approximation Methods. *Annals of Mathematics and Artificial Intelligence*. Volume 61. Issue 3. Pages 159 - 183. (2011). DOI: 10.1007/s10472-011-9260-z.
37. Changhe Yuan, Feng Cheng, Henry Dao, Markus Ettl, Grace Lin, Karthik Sourirajan. A Bayesian Framework for Supply Chain Risk Management Using Business Process Standards. Chapter in *Handbook of Integrated Risk Management in Global Supply Chains*. 2011.
38. Huang, C., Zhang, H., and Robeson, S. On the validity of commonly used covariance and variogram functions on the sphere. *Mathematical Geosciences*, Vol. 43, pp 721 – 733. (2011)
39. Gautam Rupak, and R. Higa, Model-Independent Calculation of Radiative Neutron Capture on Lithium-7, *Phys. Rev. Lett.* 106, 222501 (2011). Citations: INSPIRE (5), ADS (8)
40. Van der zwaag, J., Reed, D., Grascchel, J., Welch, D., Costanza, K., Amburn, P., Dyer, J., Moorhead, R. J., II, Zhang, S., Irby, D., & Sanyal, J. (May 2011). "FloodViz - Visual Analytics for Assessment and Interpretation of Simulated River Flooding - Presentation," 2011 Northern Gulf Institute Conference, Mobile, AL: Northern Gulf Institute.
41. Sanyal, J., Amburn, P., Zhang, S., Dyer, J., van der zwaag, J., Irby, D., & Moorhead, R. J., II. (Jun 2011). "FloodViz - A Visualization Tool for River Flow and Inundation Simulation," IEEE Visweek Poster Compendium, Providence, RI.
42. Carrel, M., X.-F. Wan, T. Ngyuen, and M. Emch. 2011. Genetic variation of highly pathogenic H5N1 avian influenza viruses in Vietnam shows both species specific and spatio-temporal associations. *Avian Diseases*, 55(4):659-666.
43. Wu, K., & Zhang, S. (Oct 2011). "Visualizing Multiple Scalar Fields with Hierarchical Topology Based on Contour Trees and Morse-Smale Complexes," IEEE VisWeek Poster Compendium, Providence, RI.

44. Zhang, G., W. Kong, W. Qi, L.-P. Long, Z. Cao, L. Huang, H. Qi, N. Cao, W. Wang, F. Zhao, M. Liao, and X.-F. Wan. 2011. Identification of an H6N6 swine influenza virus in southern China. *Infection, Genetics, and Evolution*, 11(5):1174-7.
45. Cai, Z., T. Zhang, and X.-F. Wan. 2011. Concepts and applications for influenza antigenic cartography. *Influenza and Other Respiratory Viruses*, 5 (Suppl. 1), 204–207.
46. Cai Z., Y. Duan, Y. Li, G. Lin, M. Ozden, and X.-F. Wan. 2011. IPMiner: a progenitor identifier for influenza A virus. *Influenza and Other Respiratory Viruses*, 5 (Suppl. 1), 413–415.
47. Yan, L., S. Zhang, L. Pace, F. Wilson, H. Wan, and M. Zhang. 2011. Combination of reverse transcriptase real-time polymerase chain reaction and antigen capture enzyme-linked immunosorbent assay for the detection of animals persistently infected with bovine viral diarrhoea virus. *Journal of Veterinary Diagnostic Investigation*, 23: 16-25.
48. Wan, X.-F., L. Dong, Y. Lan, L.-P. Long, C. Xu, S. Zou, Z. Li, L. Wen, Z. Cai, W. Wang, X. Li, F. Yuan, H. Sui, Y. Zhang, J. Dong, S. Sun, Y. Gao, M. Wang, T. Bai, L. Yang, D. Li, W. Yang, H. Yu, S. Wang, Z. Feng, Y. Wang, Y. Guo, R. J. Webby, and Y. Shu. 2011. Live poultry market as an important source for human H5N1 avian influenza infection in China. *J. Virol.* 85(12):13432-13438.
49. Wu, K., & Zhang, S. (Oct 2011). "A Topology Based Visualization for Exploring Data with Uncertainty," Working with Uncertainty Workshop, Providence, RI.
50. Eells, J.B., Zhang, S., Wu, R., Meyer, R.E., Coats, K.S., & Tate, D.F. (Jan 2011). "Building a Diffusion Tensor Imaging (DTI) Model of the Cat Brain to Investigate Asymmetries in the Motor Cortex and Associated White Matter," Society for Neuroscience Meeting, Washington, D.C..
51. M. J. Berg, K. R. Wilson, C. M. Sorensen, A. Chakrabarti, and M. Ahmed, "Discrete Dipole Approximation for Low-Energy Photoelectron Emission from NaCl Nanoparticles," *J. Quant. Spectros. Radiat. Transfer*, 113 p. 259-65 (2012).
52. M. J. Berg, "Optical Properties of Nanoparticle Systems: Mie and Beyond," *J. Quant. Spectros. Radiat. Transfer* 113 p. 198 (2012).
53. S. Abrahamyan et al., Measurement of the neutron radius of <sup>208</sup>Pb through parity-violation in electron scattering," *Phys. Rev. Lett* 108, 112502 (2012).
54. N. Fomin et al., New measurement of high-momentum nucleons and short-range structures in nuclei," *Phys Rev. Lett.* 108, 092502 (2012).
55. Huang et al., Beam-target double spin asymmetry A-LT in charged pion production from deep inelastic scattering on a transversely polarized He-3 target at 1.4 < Q<sup>2</sup> < 2.7 GeV<sup>2</sup>," *J. Phys Rev. Lett* 108, 052001 (2012).
56. Semi-inclusive charged-pion electroproduction on protons and deuterons: cross sections, ratios and access to quark parton model at low energies," R. Asaturyan et al., *Phys. Rev. C* 85, 015202 (2012).
57. Leading E1 and M1 contribution to radiative neutron capture on lithium-7, Gautam Rupaak and L. Fernando and R. Higa, *Eur. Phys. J. A* 48, 24 (2012). Citations: INSPIRE (2), ADS (2)
58. Cai, Z., T. Zhang, and X.-F. Wan. 2012. Antigenic distance measurements for seasonal influenza vaccine selection. *Vaccine*, 30(2):448-453.

59. Xuan, P., Y. Zhang, T. Tzeng, X.-F. Wan, and F. Luo. 2012. A quantitative structure-activity relationship (QSAR) study on glycan array data to determine the glycan binding specificities. *Glycobiology*, 22(4), 552-560.

### ***Refereed Conference Proceedings***

1. Electrochemical Society Transactions 33, 33-36, with former post-doc Ibrahim Abou Hamad, MSU CH professor David Wipf, and Florida State U. Professor Per Arne Rikvold, "A New Charging Method for Li-ion Batteries: Dependence of the Charging on the Direction of the Additional Oscillating Field"
2. R. Mehrotra, A. Dubey, S. Abdelwahed "Large Scale Monitoring and Online Analysis in a Distributed Virtualized Environment", in, 8th IEEE Conference and Work-shops on Engineering of Autonomic and Autonomous Systems (EASe 2011), Las Vegas, NV, 2011.
3. J. Shi, R. Amgai, A. Albanna, and S. Abdelwahed, "A Predictive Control Scheme for Minimizing Power Losses in Flexible Shunt Switching Compensator System", in the IEEE Power and Energy Conference at Illinois (PECI'11), Urbana, Illinois, 2011.
4. S. Srivastava, I. Banicescu, F. Ciorba, and W. Nagel, "Enhancing the Functionality of a GridSim-based Scheduler for Effective Use with Large-Scale Scientific Applications", In Proceedings of the IEEE International Symposium on Parallel and Distributed Computing (ISPDC 2011), on CD-ROM, IEEE Computer Society Press. (BEST PAPER AWARD)
5. Changhe Yuan, Brandon Malone and Xiaojian Wu. Learning Optimal Bayesian Networks Using A\* Search. In *Proceedings of the 22nd International Joint Conference on Artificial Intelligence (IJCAI-11)*. Pages 2186--2191. Barcelona, Catalonia, Spain, July 2011. (Acceptance rate: oral & poster, 17%)
6. Van der zwaag, J., Reed, D., Grascchel, J., Welch, D., Costanza, K., Amburn, P., Dyer, J., Moorhead, R. J., II, Zhang, S., Irby, D., & Sanyal, J. (May 2011). "FloodViz - Visual Analytics for Assessment and Interpretation of Simulated River Flooding - Presentation," 2011 Northern Gulf Institute Conference, Mobile, AL: Northern Gulf Institute.
7. Sanyal, J., Amburn, P., Zhang, S., Dyer, J., van der zwaag, J., Irby, D., & Moorhead, R. J., II. (Jun 2011). "FloodViz - A Visualization Tool for River Flow and Inundation Simulation," IEEE Visweek Poster Compendium, Providence, RI.
8. Wu, K., & Zhang, S. (Oct 2011). "Visualizing Multiple Scalar Fields with Hierarchical Topology Based on Contour Trees and Morse-Smale Complexes," IEEE VisWeek Poster Compendium, Providence, RI.
9. Wu, K., & Zhang, S. (Oct 2011). "A Topology Based Visualization for Exploring Data with Uncertainty," Working with Uncertainty Workshop, Providence, RI.
10. Eells, J.B., Zhang, S., Wu, R., Meyer, R.E., Coats, K.S., & Tate, D.F. (Jan 2011). "Building a Diffusion Tensor Imaging (DTI) Model of the Cat Brain to Investigate Asymmetries in the Motor Cortex and Associated White Matter," Society for Neuroscience Meeting, Washington, D.C.
11. Brandon Malone, Changhe Yuan, Eric Hansen and Susan Bridges. "Memory-Efficient Dynamic Programming for Learning Optimal Bayesian Networks," In *Proceedings of the 25th AAAI Conference on Artificial Intelligence (AAAI-11)*. Pages 1057-1062. San Francisco, CA. August 2011. (Acceptance rate: oral, 25%)

12. Brandon Malone, Changhe Yuan, Eric Hansen and Susan Bridges. Improving the Scalability of Optimal Bayesian Network Learning with Frontier Breadth-First Branch and Bound Search. In *Proceedings of the 27th Conference on Uncertainty in Artificial Intelligence (UAI-11)*. Pages 479-488. Barcelona, Catalonia, Spain, July 2011. (Acceptance rate: poster, 34%)
13. R. Mehrotra, A. Dubey, S. Abdelwahed "RFDMon: A Real-Time and Fault-Tolerant Distributed System Monitoring Approach", in, The Eighth International Conference on Autonomic and Autonomous Systems (ICAS 2012), St. Maarten, Netherlands Antilles, March 2012.
14. Nitin Sukhija, Florina Ciorba, Ioana Banicescu and Srishti Srivastava, Towards the Scalability of Dynamic Loop Scheduling Techniques via Discrete Event Simulation", Mahadevan Balasubramaniam, In *Proceedings of the IEEE International Parallel and Distributed Processing Symposium*, May 21-25, 2012, Shanghai, China, on CD-ROM, IEEE Computer Society Press.
15. Rajat Mehrotra, Ioana Banicescu and Srishti Srivastava, "A Utility Based Power-Aware Autonomic Approach for Running Scientific Applications", In *Proceedings of the IEEE International Parallel and Distributed Processing Symposium*, May 21-25, 2012, Shanghai, China, on CD-ROM, IEEE Computer Society Press.
16. Florina Ciorba, Timothy Hansen, Srishti Srivastava, Ioana Banicescu, Anthony, "A Combined Dual-stage Framework for Robust Scheduling of Scientific Applications in Heterogeneous Environments with Uncertain Availability".
17. Maciejewski, and Howard Jay Siegel, In *Proceedings of the IEEE International Parallel and Distributed Processing Symposium*, May 21-25, 2012, Shanghai, China, on CD-ROM, IEEE Computer Society Press.
18. Arindam Khaled, Changhe Yuan, Eric Hansen. Solving Limited Memory Influence Diagrams Using Branch-and-Bound Search. In *Proceedings of the International Symposium on Artificial Intelligence and Mathematics (ISAIM-12)*. January 2012



[www.ccs.msstate.edu](http://www.ccs.msstate.edu)