



The Center for Computational Sciences is a member of the College of Arts and Sciences and the High Performance Computing Collaboratory at Mississippi State University.

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 2009 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 NSF Proposal for Interdisciplinary Training for Undergraduates in Biological and Mathematical Sciences; (4) Initiating the establishment of a Center for Autonomic Computing; and (5) Eighth Mississippi State - UAB Conference on Differential Equations and Computational Simulations. This conference was dedicated to Joe E. Thompson, W.L. Giles Distinguished Professor, for his outstanding contributions to Mississippi State University.

This report will provide details of these activities/initiatives, the list of CCS Personnel, the 2009 awards and recognitions, and the 2009 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, 2009 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

CCS Personnel

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

Physics Seong-Gon Kim, Associate Director, Associate Professor Anatoli Afanasjev, Associate Professor Torsten Clay, Associate Professor Mark Novotny, Professor and Department Head Gautam Rupak, Assistant Professor Deepankgar Dutta, Assistant Professor

Electrical & Computer Engineering Sherif Abdelwahed, *Assistant 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 Edwin A. Lewis, Professor and Department Head **Steven Gwaltney**, Associate Professor

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

Statistics QiQi Lu, Assistant Professor Huiping Xu, Assistant Professor Haimeng Zhang, Assistant Professor Meng Zhao, Assistant Professor

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

Affiliated Faculty Susan Bridges, Professor, Computer Science Department Shane Burgess, Director, Life Sciences & Biological Institute 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 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, and Dr. Jagadish Singh 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 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 2: Current-Rewritable Magnetic NanoscaleMemory 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 spinflipping arrangement for nanoscale non-volatile magnetic memory cells.



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.



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

ORGANIZATION

Task 1 Task 3 Task 4 Task 2 **Optimizing Magnetic** Current-Rewritable Voltage-Rewritable Nanosensors for Title **Properties of** Nanoscale Magnetic Multiferroic Memory Chemical Warfare Hexaferrites Memory Cells Cells Agents Lead S. Kim (MSU, Phys) M. Novotny (MSU, Phys) T. Clay (MSU, Phys) J. Singh (MSU, ICET) T. Clay (MSU, Phys) S. Kim (MSU, Phys) S. Gwaltney (MSU, Chem) H. Lim (MSU, Math) S. Gwaltney (MSU, Chem) P. Ray (JSU, Chem) Team R. Shivaji (MSU, Math) S. Erwin (NRL) S. Erwin (NRL) F. Yueh (MSU, ICET) Y. Hong (UA, ECE) Y. Hong (UA, ECE) Y. Hong (UA, ECE) Postdoc 2 Postdoc (MSU) 2 Postdoc (MSU) 2 Postdoc (1 MSU + 1 UA) 1 Postdoc (MSU) 4 GRA (2 MSU + 2 UA) 4 GRA (3 MSU + 1 JSU) Student 3 GRA (MSU) 3 GRA (MSU)

Interdisciplinary team: Computational Physics, Experimental Physics, Chemistry, Mathematics, Electrical and Computer Engineering, Materials Science Education: 14 doctoral students and 7 postdocs will be involved in research each year

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)



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 Ni₈₀Fe₂₀ thin film elements
 - Recently synthesized world's smallest (< 20 nm) spherical Ba- hexaferrite nanoparticles.
- Dr. S. Erwin of NRL (Task 1 & 3) is one of the world's best experts in nanocrystal doping and theory of magnetism.





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



ECONOMIC IMPACT



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.



Of the seventy-one applications received for the 2010 REU Program, 7 students were selected from the pool of very strong applicants.



REU Program - Summer 2010 Participants:

(L to R) Helene Duke, Providence College; Justin Hansen, University of Vermont; Yicong Yong, University of Florida; Brittany Stephenson, Mississippi State University; Emily Pool, University of Arkansas; John Corring, University of Southern Mississippi; Bonnie Roberson, Mississippi State University

Biologists, computer scientists, and statisticians join to submit an NSF-UBM (National Science Foundation – Interdisciplinary Training for Undergraduates in Biological Sciences and Mathematical Sciences) proposal

Dr. Christopher Brooks led a team of members, Haimeng Zhang, Lisa Wallace, Huiping Xu and Changhe Yuan, in the submission of a UBM Group proposal **"The Landscape Genetics of Plant-Pollinator Interactions-Integrating Models and Data"**. This project aims at three year research experiences for MSU undergraduate participants. Participants will be provided a comprehensive educational exposure to mathematical biology while they are involved in research projects that address important questions in landscape genetics. This initiative is expected to greatly enhance the interaction between biologists and mathematicians at MSU.



Computer scientists and engineers join to propose the establishment of a Center for Autonomic Computing

Dr. Ioana Banicescu (PI) along with Dr. Sherif Abdelwahed (Co-PI) is planning to establish a Center for Autonomic Computing through CCS. They received an NSF planning grant and have submitted a full proposal to the NSF as well as for the Federal Initiatives Funding. The prospective activities of the Center for Autonomic Computing at Mississippi State University aim towards the development of model-driven frameworks, based on model-based or model-free approaches, for autonomic computing systems and applications.



Mathematicians host an international conference on Differential Equations and Computational Simulations.

CCS hosted an International Conference (8th Mississippi State-UAB Conference) on Differential Equations and Computational Simulations with representatives from twelve countries attending.

The primary objective of this conference 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.



The Eighth Mississippi State-UAB Conference on Differential Equations and Computations May 7-9, 2009 The Eighth Mississippi State-UAB Conference on Differential Equations and Computational Simulations was held on May 7-9, 2009, at Mi 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 Minnesota Jere Segrest, University of Alabama at Birmingham A total of 147 participants and 20 int came from 12 different countries. The 20 Joe F. Thompson dedicated to Joe F. Thompson, W. L. Giles Damager 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.



Ratnasingham Shivaji, shivaji@ra.msstate.edu • Bharat Soni, bsoni@uab.edu Jianping Zhu, jzhu@math.uta.edu • Hyeona Lim, hlim@math.msstate.edu • Roy Koomullil, rkoomul@uab.edu

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Conference Participants' Comments:

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.

Alfonso Castro, Harvey Mudd College

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

Jerry Goldstein, University of Memphis

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.

Nicolae Tarfulea, Purdue University Calumet

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.

Georg Hetzer, Auburn University

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!

Anatoli F. Ivanov, Penn State University

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!

Zhifu Xie, Virginia State University

CCS Awards and Recognition



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 2010.



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".

Center for Computational Sciences

CCS Awards and Recognition



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 planning grant to start 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

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	\$212,000	Afanasjevs	Awarded (12/15/06 - 11/14/09)
Environment Canada	Changepoint Estimation for Canadian Sky-Cloudiness Frequencies Using a Temporal Continuation-Ratio Logit Model	\$20,000	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	\$507,111	Clay	Awarded (09/01/08 - 8/31/10)
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)
DOE	Nuclei at Extreme Conditions: A Relativistic Study	\$222,000	Afanasjevs	Awarded (11/15/09 - 11/14/12)
MS Soybean Promotion Board	Identifying Full-Length Open Reading Frames of Genes involved in Interactions between Soybean and Nematodes	\$35,000	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 Multivariate Probit Analysis	\$10,000	Xu	Awarded (01/01/10 - 12/31/10)

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	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
US Department of Energy (12/01/08)	Few-and Many-Body Nuclear Theory from QCD	\$383,461	Rupak	Pending
National Science Foundation (01/20/09)	GEPR: Identification of Gene Regulatory Networks Involved in Resistance as Identified by Laser Capture Microdissection and FLX-454 Sequencing of RNA Isolated from Nematode Feeding Sites	\$869,986	Klink	Pending
DOE (09/01/09)	Universality, Nuclear Physics and QCD	\$843,338	Rupak	Pending
National Science Foundation (12/15/09)	Efficient Numerical Methods for Variational Image Restoration and Segmentation	\$217,702	Lim	Pending
National Science Foundation (09/30/09)	Composition Markov Chains of Multinomial Type	\$33,165	Zhang	Pending
National Science Foundation (07/24/09)	Collaborative Research: Magnolia grandiFLORA: A digital Herbarium of Collections in Mississippi	\$677,146	L. Wallace, C. Brooks, G. Ervin	Pending
NIH (09/24/09)	Early Detection of Myocardial Infraction: A 3D Diffusion Tensor MRI Study on Heart Fiber Architecture	\$418,476	Zhang	Pending
National Science Foundation (10/31/09)	Materials Inspired by Network Theory	\$488,960	Novotny	Pending
National Science Foundation (10/31/09)	Tailoring Magnetic Properties of Hexagonal Ferrites	\$494,638	Kim	Pending
National Science Foundation (01/13/10)	A Mechanical and Computational Model of the Unicellular Green Algae Chlamydomonas	\$73,955	Yang	Pending
National Science Foundation (02/01/10)	Characterization of cpDNA SSR's in Lotus for inferring phylogeographic patterns on the Channel Islands	\$14,401	Wallace	Pending
National Science Foundation (02/11/10)	UBM Group: The Landscape Genetics of Plant-Pollinator Interactions – Integrating Models and Data	\$237,780	Brooks, Zhang, Wallace, Xu, Yuan	Pending
National Science Foundation (03/06/10)	Center for Autonomic Computing at Mississippi State University	\$274,789	Banicescu, Abdelwahed	Pending
National Science Foundation (06/01/10)	EMSW21-RTG Research Training in Partial Differential Equations with applications in Biology and Material Science	\$2,126,807	Lim, Shivaji, Yang, Yarahmadian	Pending

Other CCS Recent Proposals

Sponsor	Project Title	Personnel
Ultralife Corporation	Confirmation and Development of a Fast- Charging Method for Lion-Cells	Novotny, Wipf
National Science Foundation	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	Zhang, Lu, Jin, Ling
National Science Foundation (10/30/08)	4D CFD; A Spatiotemporal Approach to Fluid Dynamics	Walters, Banicescu, Bur green
DOE	Integrated Simulations and Experiments to Develop Reforming Catalyst for Renewable Hydrogen Production from Glycerin	Gwaltney, Kim, Kim, Fernando
National Science Foundation	Ecological Influences on the Evolutionary Diversification of Orchids: A Multidisciplinary Study of Landscape Genetics, Floral Morphology and Selection in Plantanthera Dilatata	Wallace
National Science Foundation (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
National Science Foundation	CSUMS: Undergraduate Research and Training in Differential Equations and their Applications	Kim, Lim, Janus, Shivaji, Park
National Science Foundation	Major research Instrumentation (jointly with LSBI, IDB, and CCS)	Burgess, Banicescu, Bridges, Lawrence, Peterson

Patents

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

Refereed Journal Publications

S. Abdelwahed, R. Su, J. Bai and N. Kandasamy, "On the Application of Predictive Control Techniques for Adaptive Performance Management of Computing Systems", IEEE Transactions on Network and Service Management, vol. 6, no.4, 212-225, 2009.

A. Dubey, R. Mehrotra, S. Abdelwahed and A. Tantawi, "Performance Modeling of Distributed MultiTier Enterprise Systems", ACM Performance Evaluation Review, vol.37,no.2,9-11, Sept 2009.

G. Madl, S. Pasricha, N. Dutt and S. Abdelwahed, "Crodd-abstraction Functional Verification and Performance Analysis of Chip Multiprocessor Designs", IEEE Transaction on Industrial Electronics, Special Section on Real-Time and Networked Embedded Systems, vol.5, no.3, 241-256, August 2009.

S. Abdelwahed, G. Karsai, N. Mahadevan and S.C. Ofsthun, "Practical considerations in systems diagnosis using timed failure propagation graph models", IEEE Transactions on Instrumentation and Measurement, vol. 58, no.2, 240-247, 2009.

G. A. Lalazissis, S. Karatzikos, R. Fossion, D.P. Arteaga, A.V. Afanasjev and P. Ring, "The effective force NL3 revisited", Physics Letters, B 671, 36-41, 2009.

H. Abusara and A.V. Afanasjev, "Hyperdeformation in the Cd isotopes: A miscroscopic analysis", Physical Review C 79, 024317, 1-7, 2009.

Q.A. Ijaz, W.C. Ma, H. Abusara, A.V. Afanasjev, Y.B. Xu, R.B. Yadav, Y.C. Zhang, M.P. Carpenter, R.V.F. Janssens, T.L. Khoo, T. Lauritsen and D.T. Nisius, "Observation of excited superdeformed bands in ¹⁵⁴Dy and cranked relativistic mean field interpretation", Physical Review, C 80, 034322, 1-7, 2009.

H.B. Jeppesen, R.M. Clark, K.E. Gregorich, A.V. Afanasjev, M.N. Ali, J.M. Allmond, C.W. Beausang, M. Cromaz, M.A. Deleplanque, I. Dragojevic, J. Dvorak, P.A. Ellison, P. Fallon, M.A. Garcia, J.M. Gates, S. Gros, I.Y. Lee, A.O. Macchiavelli, S.L. Nelson, H. Nitsche, L. Stavsetra, F.S. Stephens and M. Wiedeking, "High-K Multi-quasiparticle States and Rotational Bands in ¹⁰³Lr²⁵⁵", Physical Review, C 80, 034324 1-4, 2009.

R.D. Herzberg, S. Moon, S. Eeckhaudt, P.T. Greenlees, P.A. Butler, T. Page, A.V. Afanasjev, N. Amzal, J.E. Bastin, F. Becker, M. Bender, B. Bruyneel, J.F.C. Cocks, I.G. Darby, O. Dorvaux, K. Eskola, J. Gerl, T. Grahn, C. Gray-Jones, N.J. Hammond, K. Hauschild, P.H. Heenen, K. Helariutta, A. Herzberg, F. Hessberger, M. Houry, A. Hurstel, R.D. Humphreys, G.D. Jones, P.M. Jones, R. Julin, S. Juutinen, H. Kankanpaa, H. Kettunen, T.L. Khoo, W. Korten, P. Kuusiniemi, Y. LeCoz, M. Leino, A.P. Leppanen, C.J. Lister, R. Lucas, M. Muikku, P. Nieminen, M. Nyman, R.D. Page, T. Page, J. Pakarinen, A. Pritchard, P. Rahkila, P. Reiter, M. Sandzelius, J. Saren, C. Schlegel, C. Scholey, C. Theisen, W.H. Trzaska, J. Uusitalo, A. Wiens and H.J. Wollersheim, "Structure of rotational bands in ²⁵³No", European Physical Journal, A42, 333-337, 2009.

I. Banicescu, F. Ciorba and R. Carino, "Towards the Robustness of Dynamic Loop Scheduling on Large-Scale Heterogeneous Distributed Systems", In Proceedings of the IEEE International Symposium on Parallel and Distributed Computing (ISPDC 2009), on CD-ROM, IEEE Computer Society Press.

P. J. Vardon, I. Banicescu, P.J. Cleall, H.R. Thomas and R.N. Philip, "Coupled Thermo-Hydro-Mechanical Modeling: A New Parallel Approach", In Proceedings of the IEEE International Symposium on Parallel and Distributed Computing (ISPDC 2009), on CD-ROM, pp. 1-9, IEEE Computer Society Press.

V.J. Alarcon, W. McAnally, G. Ervin and C.P. Brooks, "Using MODIS Land-Use/Land-Cover Data and Hydrological Modeling for Estimating Nutrient Concentrations", In: Computational Science and Its Applications - ICCSA 2010 (Taniar, D.; Gervasi, O.; Murgante, B.; Pardede, E.; Apduhan, B.O. Eds.), Lecture Notes in Computer Science 6016. Springer-Verlag, Berlin, 501-514, 2009.

R.T. Clay, S. Mazumdar and H. Li, "Local singlets, frustration, and unconventional superconductivity in the organic charge-transfer solids," Physica B, volume 404, issue 3-4, 487-489, 2009.

R.T. Clay, H. Li and S. Mazumdar, "Bipolaron density-wave driven by antiferromagnetic correlations and frustration in organic superconductors", Dec 11 2009, Physica B, doi:10.1016/j.physb.2009.11.091.

S. Mazumdar, R.T. Clay and H. Li, "From valence bond solid to unconventional superconductivity in the organic charge-transfer solids," Synthetic Metals, volume 159, 2419-2421, 2009.

J. Seely, D. Dutta, et al., "*New Measurement of the European Muon Collaboration Effect in Very Light Nuclei*", Phys. Rev. Lett, vol., 103, 202301, 2009.

D. Hasell, D. Dutta, et al., "The BLAST Experiment", Nucl. Instrum. Meth. A603, 247, 2009.

S. P. Malace, D. Dutta, et al., "*Applications of quark-hadron duality in the F2 structure function*", Phys. Rev. C, vol 80, 035207, 2009.

A. N. Vilano, D. Dutta, et al., "*Electroproduction in the Resonance Region at High Q* 2 ", Phys. Rev. C, vol 80, 035203, 2009.

M. M. Dalton, D. Dutta, et al., *"Electroproduction of eta Mesons at the S11 (1535) Resonance Region at High Momentum Transfers"*, Phys. Rev. C, vol 80, 015205, 2009.

Q. Ye, H. Gao, W. Zheng, D. Dutta, F. Dubose, R. Golub, P. Huffman, C. Swank and E. Korobkina, "*Relaxation of Spin Polarized He-3 in Mixtures of He-3 and He-4 at about 330 mK*", Phys. Rev. A, vol 80 023403, 2009.

W. Chen, T. Mibe, D. Dutta, et al. "*Measurement of the Differential Cross Section for the Reaction gamma n -> pi^{-} p from Deuterium*", Phys. Rev. Lett., vol 103, 012301, 2009.

P. Bosted, J. Dunne, D. Dutta, et al. "*Search for sub-threshold photoproduction of J/Psi mesons*", Phys. Rev. C, Vol 79, 015209, 2009.

D. Hossain, S. R. Gwaltney, C. U. Pittman, Jr. and S. Saebo, "Insertion of transition metal atoms and ions into the nanoscale dodecahedral silsesquioxane (T_{12} –POSS) cage: Structures, stabilities and electronic properties," Chem. Phys. Lett. 467, 348–353, 2009.

J. A. Yancey, M. A. Novotny and S. R. Gwaltney, "Small Pure Carbon Molecules with Small World Networks using Density Functional Theory Simulations", Int. J. Modern Phys. C 20, 1345-1356, 2009.

R. Q. Hu, W. Hu, M. Jin and Y. Qian, "Wavelength Retuning without Service Interruption in an All-Optical Survivable Network," International Journal of Communication Systems, v22/6, FEB, 719-738, 2009.

R. Kaul, Y. Yun, and S.G. Kim, "Ranking billions of web pages using diodes", Commun. ACM., 52 (8), 132-136, 2009.

S.G. Kim, M. F. Horstemeyer, M. I. Baskes, M. Rais-Rohani, S. Kim, B. Jelinek, J. Houze, A. Moitra and L. Liyanage, "Semi-empirical Potential Methods for Atomistic Simulations of Metals and Their Construction Procedures," J. Eng. Mater. Technol., 131 (4), 2009, 041210 [9 pages].

J. Jalli, Y.K. Hong, S. Bae, G. S. Abo, J.J. Lee, J.C. Sur, S.H. Gee, S.G. Kim, S.C. Erwin and A. Moitra, "Conversion of Nano-sized Spherical Magnetite to Spherical Barium Ferrite Nanoparticles for High Density Particulate Recording Media," IEEE Trans. Magn. 45(10), 3590-3593, 2009.

A.N. Yancey, S.G. Kim and J.T. Foley, "Visualizing Complicated Quantum Mechanical Behavior From Simple 2-D Potentials Using WebTOP," International Journal of Modern Physics C, 20 (9), 1431-1441, 2009.

J. Choi, S.G. Kim, J. Lee and Y.S. Choi, "Agent-Based Evacuation Simulation for Building Structure Evaluation," GIScience & Remote Sensing, 46(4), p. 1-18 2009.

R. Balestrini, J. Gómez-Ariza, V.P. Klink and P. Bonfante, "Application of Laser Microdissection (LM) in plant pathogenic and symbiotic interactions", Journal of Plant Interactions 4: 81-92, 2009.

V.P. Klink, P. Hosseini, M. H. MacDonald, N. Alkharouf and B.F. Matthews, "Populationspecific gene expression in the plant pathogenic nematode Heterodera glycines exists prior to infection and during the onset of a resistant or susceptible reaction in the roots of the Glycine max genotype", Peking. BMC-Genomics, 10: 111,2009.

V.P. Klink, K.H. Kim, V.E. Martins, M.H. MacDonald, H.S. Beard, N.W. Alkharouf, S.K. Lee, S.C. Park, B.F. Matthews, "A correlation between host-mediated expression of parasite genes as

tandem inverted repeats and abrogation of the formation of female Heterodera glycines cysts during infection of Glycine max", Planta, 230: 53-71, 2009.

V.P. Klink , P. Hosseini, P. Matsye , N. Alkharouf and B.F. Matthews, "A gene expression analysis of syncytia laser microdissected from the roots of the Glycine max (soybean) genotype PI 548402 (Peking) undergoing a resistant reaction after infection by Heterodera glycines (soybean cyst nematode)", Plant Molecular Biology, 71: 525-567,2009.

V.P. Klink and B.F. Matthews, "Emerging approaches to broaden resistance of soybean to soybean cyst nematode supported by gene expression studies", Plant Physiology, 151:1017-1022, 2009.

H. Lim and S. Kim, "Fourth-order partial differential equations for effective image denoising," Electron. J. Differ. Equ., 17, 107-121,2009.

H. Lim, H. Rhee, M. Horstemeyer, H. Hwang, H. El Kadiri and W. Trim, "A study on the structure and mechanical behavior of the Terrepene Carolina carapace: a pathway to design bio-inspired synthetic composites," Materials Sciences and Engineering C, 29, 2333-2339, 2009.

M. L. Guerra, M.A. Novotny, H. Watanabe and N. Ito, "Efficiency of Rejection-Free Methods for Dynamic Monte Carlo Studies of Off-lattice Interacting Particles", Physical Review E, vol 79, article 026706 [6 pages] 2009.

S.H. Thompson, G. Brown, A.D. Kuhnle, P.A. Rikvold and M.A. Novotny, "Resolutiondependent Mechanisms for Bimodal Switching-time Distributions in Simulated Fe Nanopillars", Physical Review B, vol. 79, article 024429 [9 pages] 2009. (Artwork chosen for Jan. 2009, Physical Review B, Kaleidoscope)

P.A. Rikvold, I. A. Hamad, T. Juwono, D.T. Robb and M.A. Novotny, "Applications of Computer Simulations and Statistical Mechanics in Surface Electrochemistry", in Modern Aspects of Electrochemistry, vol. 44, edited by M. Schlesinger (Springer-Verlag, Berlin Heidelberg, 2009), Chapter 4, pages 131-149 (invited book chapter).

J. A. Yancey, M.A. Novotny and Steven R. Gwaltney, "Small Pure Carbon Molecules with Small-World Networks using Density Functional Theory", International Journal of Modern Physics C, volume 20, pages 1345-1356, 2009.

M.A. Novotny and A. Kolakowska, "Mixing Different Random Depositions in Surface Growth Models", International Journal of Modern Physics C, volume 20, pages 1377-1385, 2009.

I.I. Levin, D.C. Outlaw, H. Vargas and P. G Parker, "Plasmodium blood parasite found in endangered Galapagos penguins (Spheniscus mendiculus)", Biological Conservation 142: 3191-3195, 2009.

D.C. Outlaw and R. E. Ricklefs, "On the phylogenetic relationships of haemosporidian parasites from raptorial birds (Falconiformes and Strigiformes)", Journal of Parasitology, 95: 1171-1176, 2009.

G. Voelker, S. Rohwer, D. C. Outlaw and R. C. K. Bowie, "Repeated trans-Atlantic dispersal catalyzed a global songbird radiation", Global Ecology and Biogeography, 18:41-49, 2009.

G. Rupak and T. Schaefer, "Density Functional Theory for non-relativistic Fermions in the Unitarity Limit", Nucl. Phys. A, 816, 52, 2009.

J. Ali, D. Perry, S. Sasi, J. Schaefer, B. Schilling, R. Shivaji and M. Williams, "Population Dynamics with Symmetric and Asymmetric Harvesting", Electronic Journal of Qualitative Theory of Differential Equations, Special Edition I,No.2, 1-16,2009.

J. Ali and R. Shivaji, "Multiple positive solutions for a class of p-Laplacian systems with multiple parameters and combined nonlinear efforts", Differential Integral Equations, Vol.22 (7-8), 669-678, 2009.

E.K. Lee, R. Shivaji and J. Ye, "Subsolutions: A Journey from Positone to Infinite Semipositone Problems", Proceedings of the 7th Mississippi State UAB Conference for Differential Equations and Computational Sciences, Electronic Journal for Differential Equations Conf. Series.17, 123-131, 2009.

A. Jaffar, R. Shivaji and K. Wampler, "Population Models with Diffusion, Strong Allee Effect and Constant Yield Harvesting", J. Math. Anal. Appl., 352, 907-913, 2009.

E.K. Lee, J. Ye and R. Shivaji, "Classes of infinite semipositone systems", Proc. Royal Soc. Edin, 139A ,853-865,2009.

E.K. Lee, R. Shivaji and J. Ye, "Positive Solutions for Elliptic Equations Involving Nonlinearities with Falling Zeroes", Applied Mathematic Letters, Vol.22, No.6, 846-851,2009.

L.E. Wallace, S.G. Weller, W.L. Wagner, A.K. Sakai and M. Nepokroeff, Phylogeographic patterns and demographic history of Schiedea globosa (Caryophyllaceae) on the Hawaiian Islands. American Journal of Botany, 96: 958-967, 2009.

L.E. Wallace and K. Helenurm, "Has herbivory negatively impacted the flora of the California Channel Islands? Insights from Crossosoma californicum (Crossosomataceae)", International Journal of Plant Sciences, 170: 311-322, 2009.

P.H. Jones, L.E. Wallace and H.B. Bitten, "Isolation and characterization of 11 microsatellite loci from Oropsylla hirsuta, a common vector of sylvatic plague", Molecular Ecology Resources, 9: 1041-1044, 2009.

M.S. Furches, L.E. Wallace and K. Helenurm, "High genetic divergence characterizes populations of the endemic plant Lithophragma maximum (Saxifragaceae) on San Clemente Island", Conservation Genetics, 10: 115-126, 2009.

S.A. Pearl, M.E. Welch and D.E. McCauley, "Mitochodrial heteroplasmy and paternal leakage in natural populations of Silene vulgaris, a gynodioecious plant", Molecular Biology and Evolution, 26: 537-545, 2009.

H. Xu and Craig, B.A., "A probit latent class model with general correlation structures for evaluating accuracy of diagnostic Tests". *Biometrics*, 65 (4): 1145-1155, 2009.

L. Goldstein and H. Zhang, "Efficiency Calculations for the Maximum Partial Likelihood Estimator in Nested-Case Control Sampling". Bernoulli, 15, 569 – 597, 2009.

J. Sanyal, S. Zhang, G. Bhattacharya, P. Amburn and R. Moorhead, "A User Study to Compare Four Uncertainty Visualization Methods for 1D and 2D Datasets", IEEE Transactions on Visualization and Computer Graphics, 15(6):1209-1218, 2009.

W. Chen, Z. Ding, S. Zhang, A.M. Brandt, S. Stephen Correia, H. Qu, J.A. Crow, D.F. Tate, Z. Yan and Q. Peng, "A Novel Interface for Interactive Exploration of DTI Fibers", IEEE Transactions on Visualization and Computer Graphics, 15(6):1449-1456, 2009.

S. Yarahmadian and K. Zumbrun, "Pointwise Green Function Bounds and Long-Time Stability of Large-Amplitude Noncharacteristic Boundary Layers", SIAM J. Math. Anal., Volume 40, Issue 6, 2328-2350, 2009.

Refereed Conference Proceedings/Posters

S. Abdelwahed and G. Karsai, "Failure Prognosis Using Timed Failure Propagation Graphs", in the International Conference of the Prognostics and Health Management Society 2009), San Diego, CA 2009.

T. Morris, A. Srivastava, B. Reaves, K. Pavurapu, S. Abdelwahed, R. Vaughn, W. McGrew and Y. Dandass, "Engineering Future Cyber-Physical Energy Systems: Challenges, Research Needs, and Roadmap", the 2009 IEEE North American Power Symposium, Starkville, MS, Oct. 2009.

J. Bai and S. Abdelwahed, "Efficient Algorithms for Performance Management of Computing Systems", the 4th International Workshop on Feedback Control Implementation and Design in Computing Systems and Networks (FEBID 2009), San Francisco, CA, April 2009.

A. Dubey, D. Riley, S. Abdelwahed and Ted Bapty, "Modeling and Analysis of Probablistic Timed Systems", 16th Annual IEEE International Conference on the Engineering of Computer Based Systems (ECBS), San Francisco, CA, April 2009.

G. Madl, N. Dutt, S. Abdelwahed and S. Rajan, "A conservative approximation method for the verification of preemptive scheduling using timed automata", in Proc. 15th IEEE Real-Time and Embedded Technology and Applications Symposium (RTAS'09), San Francisco, California, 2009.

A. Dubey, G. Karsai and S. Abdelwahed, "Compensating for Timing Jittr in Computing Systems with General-Purpose Operating Systems", 12th IEEE International Symposium on Object/component/service-oriented Real-time distributed Computing (ISORC 2009), Tokyo, Japan, March 2009.

Z. Zhang and M. Jin, "Analysis of Capacity-Constrained Sequential Auctions in Duopoly Market Environment," Proceedings of the IEEE International Conference on Industrial Engineering and Engineering Management (IEEM 2009), Hong Kong, China, Dec 2009.

Y. Ling, M. Jin, M. Hilliard and J. Usher, "A study of Real-Time Identification and Monitoring of Barge-Carried Hazardous Commodities," Proceedings of the 17th International Conference on Geoinformatics, Fairfax, VA, Aug 2009.

C. Morris and M. Jin, "A Semi-Markov Decision Process for Transshipment of Critical, Slow-Moving Medical Goods," Proceedings of Industrial Engineering Research Conference, Miami, FL. May 2009.

C. Yuan, X. Liu, T.C. Lu and H. Lim, "Most Relevant Explanation: Properties, Algorithms, and Evaluations", the 25th Conference on Uncertainty in Artificial Intelligence (UAI-09), June 18-21, Montreal, Canada.

C. Yuan and E. Hansen, "Efficient Computation of Jointree Bounds for Systematic MAP Search", Twenty-First International Joint Conference on Artificial Intelligence (IJCAI-09), Pasadena, CA. 2009.

C. Yuan, "Some Properties of Most Relevant Explanation", Twenty-First International Joint Conference on Artificial Intelligence ExaCt Workshop (ExaCt-09), Pasadena, CA. 2009.

W. Chen, S. Zhang, S. Correia and D. F. Tate, "Visualizing Diffusion Tensor Imaging Data ith Merging Ellipsoids", IEEE Pacific Visualization Symposium, Beijing, China, April 2009.

S. Zhang, Z. Yan, W. Chen, J. Crow, R. McLaughlin, R. Cooper, X. Yang and Jun Liao, "Muscle fiber visualization from Diffusion Tensor Imaging data", BMES, October 2009.

K. Wu, S. Zhang, P. Amburn and R. J. Moorhead, "Using A LIC-like FlowVis Technique to Visualize Hurricanes", IEEE Visualization 2009, Atlantic City, NJ.

J. Sanyal, P. Amburn, S. Zhang, P. J. Fitzpatrick and R.J. Moorhead, "3D Immersive Visualization and Evaluation of Mesoscale Model Outputs Simulating Hurricane Lili's (2002) Rapid Weakening", Oceans 2009, Biloxi, MS.



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