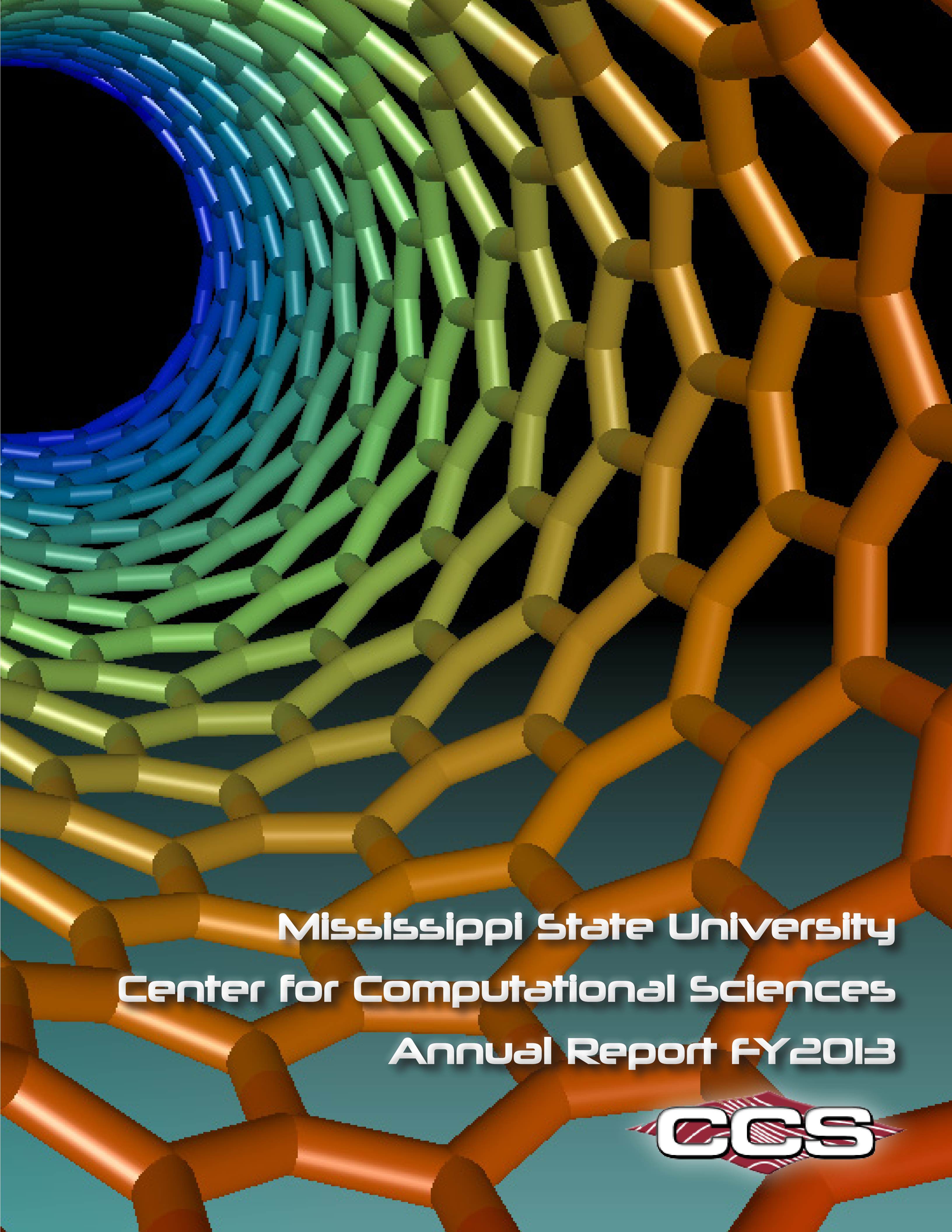


Mississippi State University
Center for Computational Sciences
Annual Report FY2013

CCS

Director's Note

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

The major research activities/initiatives of CCS 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-Tc superconductivity phenomena in layered organic and inorganic materials; (5) DOE funded project on rare-earth-free nanostructure permanent magnets; and (6) Image processing in bio-inspired materials design. 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 Materials Research Science and Engineering Centers (MRSEC).

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, this year has been a successful year for CCS. We look forward to building on this platform, to achieve greater excellence in coming years.

Seong-Gon Kim

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

Mission

To foster interdisciplinary research in both the fundamental understanding of and application of all the natural sciences. In particular, to model and develop integrated computational environments and crosscutting tools that allow a comprehensive, cross-disciplinary approach to problem-solving.

CCS Personnel

Director: Seong-Gon Kim, Professor, Physics and Astronomy
Associate Director: Hyeona Lim, Associate Professor, Mathematics and Statistics

<u>Biological Sciences</u>
Christopher Brooks, *Associate Professor*
Vincent Klink, *Assistant Professor*
Lisa Wallace, *Associate Professor*

<u>Chemistry</u>
Steven Gwaltney, *Associate Professor*

<u>Computer Science and Engineering</u>
Ioana Banicescu, *Professor*
Song Zhang, *Associate Professor*

<u>Electrical & Computer Engineering</u>
Sherif Abdelwahed, *Assistant Professor*
Yaroslav Koshka, *Professor*

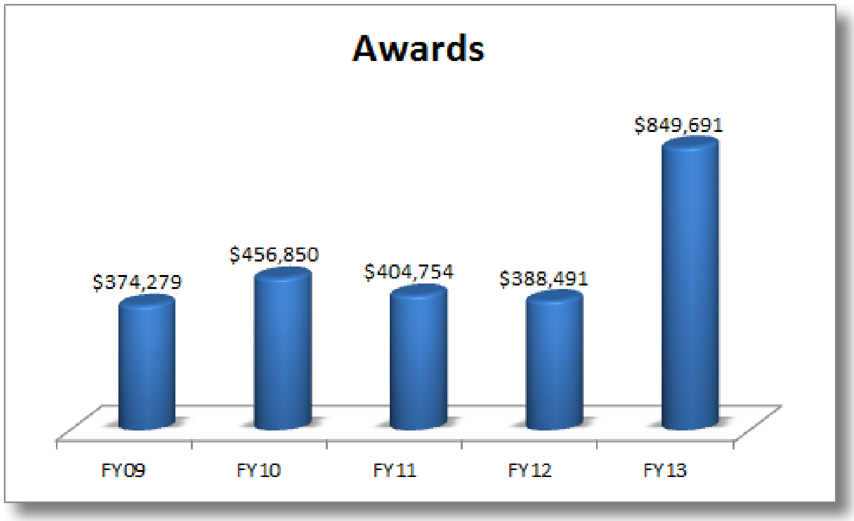
<u>Industrial and Systems Engineering</u>
Hugh Medal, *Assistant Professor*

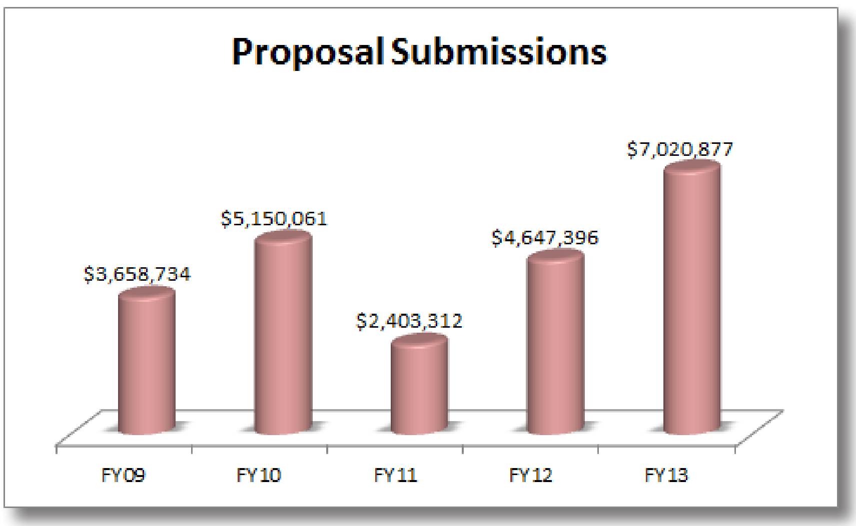
<u>Mathematics and Statistics</u>
Seongjai Kim, *Associate Professor*
Hyeona Lim, *Associate Professor*
Suzanne Shontz, *Assistant Professor*
Jonathan Woody, *Assistant Professor*
Xingzhou Yang, *Assistant Professor*
Shantia Yarahmadian, *Assistant Professor*

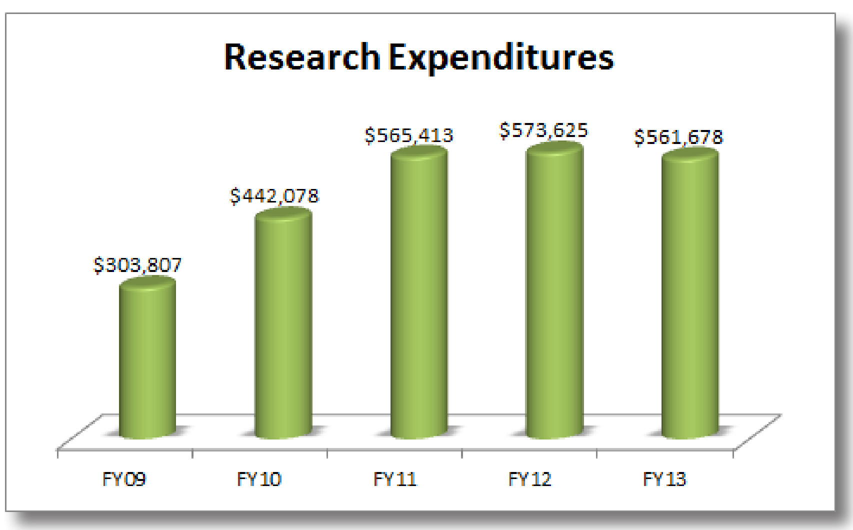
<u>Physics and Astronomy</u>
Anatoli Afanasjev, *Professor*
Matthew J. Berg, *Assistant Professor*
Torsten Clay, *Associate Professor*
Dipankgar Dutta, *Associate Professor*
Seong-Gon Kim, *Professor*
Mark Novotny, *Professor and Department Head*
Gautam Rupak, *Assistant Professor*
Jinwu Ye, *Associate Professor*

<u>College of Veterinary Medicine, Basic Sciences</u>
Henry X.-F. Wan, *Associate Professor*

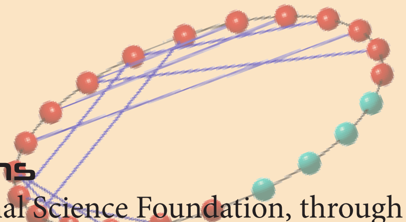
Research Activities





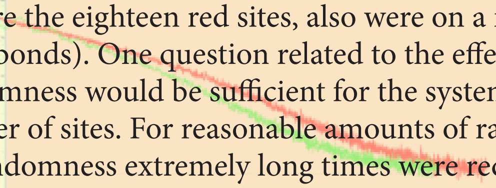


Research Highlights



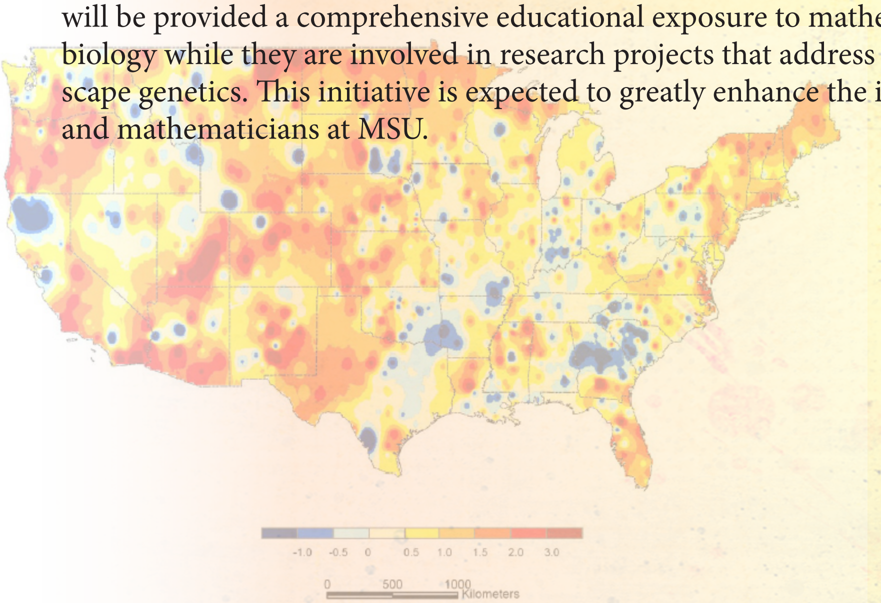
Equilibration for Classical and Quantum Systems

The work described below is supported in part by a grant from the National Science Foundation, through the Division of Materials Research. Two papers by Prof. Novotny published in the last year examined how a subsystem of an isolated physical system approaches what can be regarded as thermal equilibrium. The work was performed with collaborations in Germany, The Netherlands, and Japan. One study was for classical models, ones where Newton's equations describe the time evolution of the system. The other was for quantum systems, where the time-dependent Schrödinger equation describes the time evolution of the system. The figures are from the study of a quantum system, published in Physical Review A. The study was very computationally intensive. For example, once curve in the article required 300,000 core hours on an IBM 16384 BG/P (Blue Gene P) using 1024 Gigabytes of memory. A general case was considered theoretically and definite predictions of how quantum entanglement changes with the size of the quantum bath were obtained. One example system studied in the paper is shown, namely a one-dimensional ring of quantum spins ½ particles, but with only a small number of spins measured (the four cyan sites in the figure). The bath, in the figure the eighteen red sites, also were on a ring, and could have small-world connections between sites (the blue bonds). One question related to the effects of randomness, with the prediction that any small amount of randomness would be sufficient for the system to go to the theoretically predicted value, which depends on the number of sites. For reasonable amounts of randomness this is the case as shown in the graph. However for small randomness extremely long times were required before the system approached the theoretically predicted value. In particular the red and blue curves for small randomness do relax to the theoretical value, but as shown only for very long times. The time development of all the eigenvalues of the quantum density also had a physical interpretation, and led to very interesting curves such as the one shown.

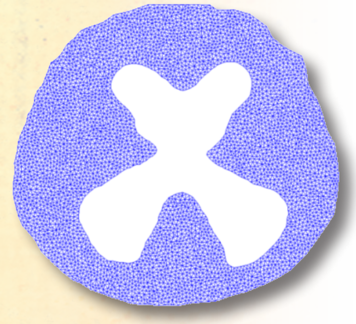


Landscape Genetics of Plant-Pollinator Interactions-Integrating Models and Data

This project led by Prof. Christopher Brooks aims at providing 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.



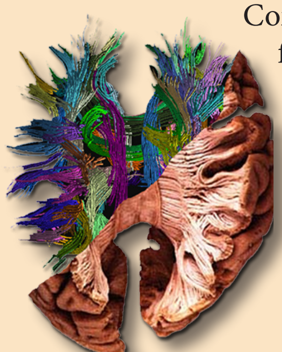
Parallel Dynamic Meshing Techniques for Simulation-Assisted Medical Interventions



The overall goal of this NSF CAREER project led by Prof. Suzanne Shontz is to research and develop parallel dynamic meshing algorithms, theory, and software for use in the design of patient-specific medical interventions, such as improved prevention of pulmonary embolism and treatment of hydrocephalus. Pulmonary embolism is a blockage in one or more arteries of the lungs usually caused by a blood clot which has broken free from a deep vein, such as the inferior vena cava (IVC), and traveled to the lungs. Hydrocephalus is a neurological disease in which excess fluid accumulates in the brain, causing the ventricles of the brain to swell, and often causing brain damage. Current simulations of blood clot entrapment by IVC filters and evolution of the brain ventricles in hydrocephalus treatment are of low accuracy. In collaborations with researchers at Penn State, the University of Utah, the University of Waterloo, Lawrence Livermore National Laboratory, and Mississippi State, we are developing novel, parallel dynamic meshing algorithms to generate anatomically accurate patient-specific meshes which arise in such simulations. Our parallel dynamic meshing algorithms are used for mesh warping and mesh quality improvement problems that arise based on the patients and medical devices in these simulations. The algorithms will be encapsulated in the form of a parallel dynamic meshing toolkit for use in simulation-assisted medical interventions, as well as numerous other applications, and is being developed for use on a distributed-memory parallel architecture.

Center for Autonomic Computing

Prof. Ioana Banicescu and Sherif Abdelwahed 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.

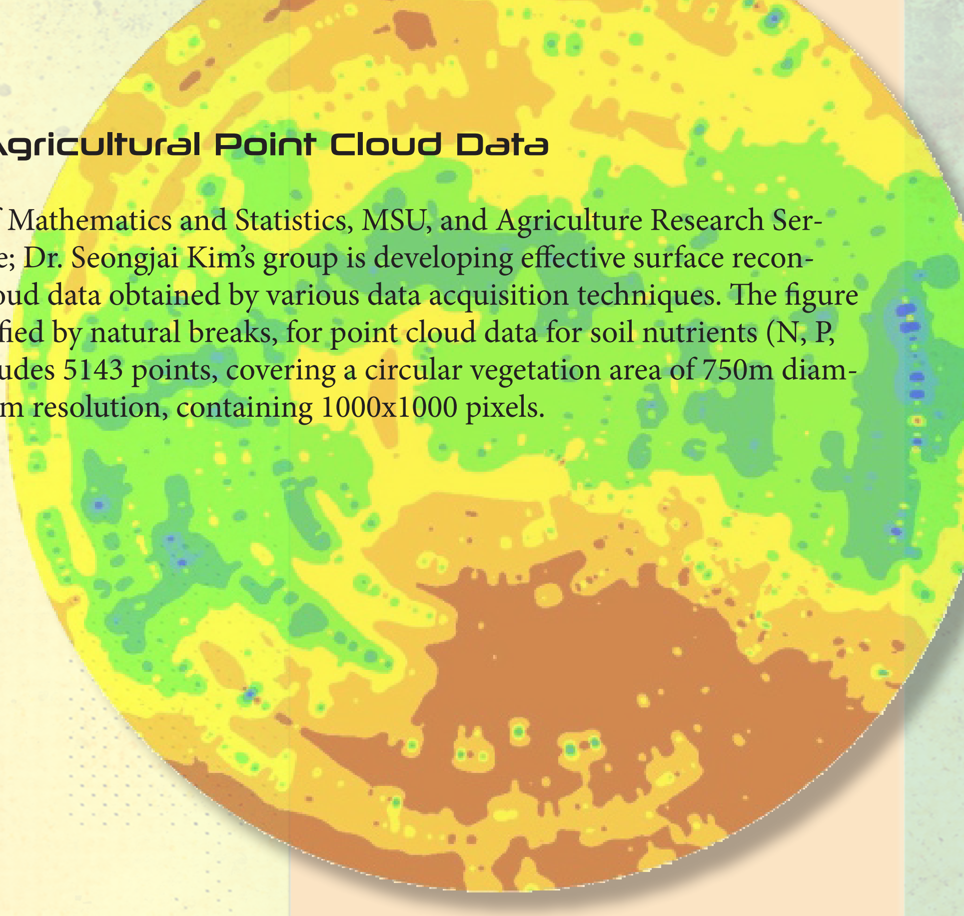


cac

Center for Cloud and Autonomic Computing
Fall 2012 Semiannual Meeting
December 10 & 11, 2012
Mississippi State University

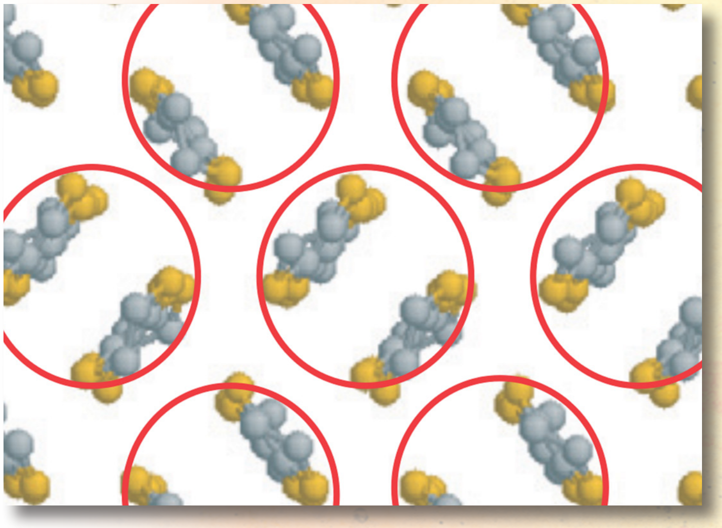
Surface Reconstruction for Agricultural Point Cloud Data by Curvature Interpolation

As a joint project between the Department of Mathematics and Statistics, MSU, and Agriculture Research Service, United States Department of Agriculture; Dr. Seongjai Kim's group is developing effective surface reconstruction algorithms for agricultural point cloud data obtained by various data acquisition techniques. The figure below shows the reconstructed surface, classified by natural breaks, for point cloud data for soil nutrients (N, P, K), acquired in March 2013. The data set includes 5143 points, covering a circular vegetation area of 750m diameter in Mississippi Delta. The image is in 0.75m resolution, containing 1000x1000 pixels.



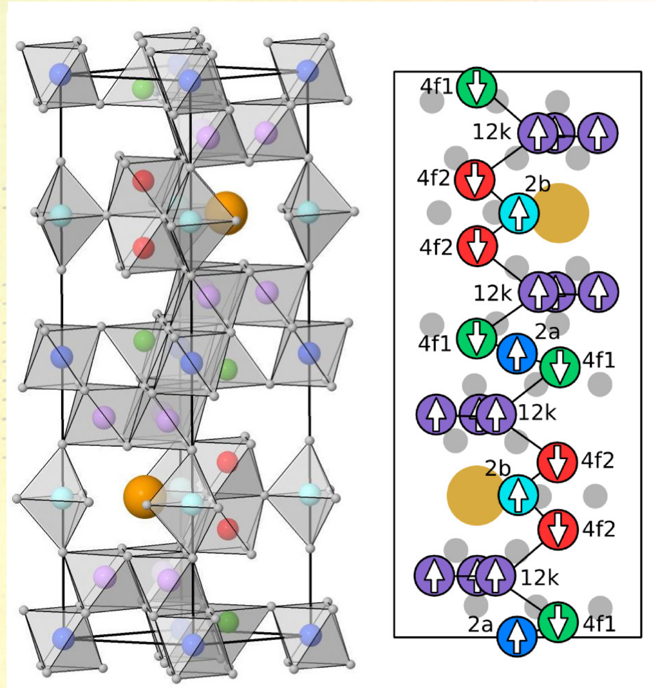
Theory of Layered Organic and Inorganic Materials with Charge-spin Frustration

In a frustrated material the lattice arrangement prevents local energy constraints from being satisfied, leading to a large degeneracy of quantum states and highly unusual electronic properties. Most theoretical work to understand frustration has been carried out on quantum spin models where charge degrees of freedom have been frozen out. In this project led by Prof. Torsten Clay, CCS researchers are investigating materials with lattice frustration where instead charge as well as spin degrees of freedom remain important at low temperatures. One application is to the two-dimensional organic superconductors κ-(BEDT-TTF)2X. In these materials the occurrence of antiferromagnetism indicates that electron-electron interactions are significant. An effectively 1/2-filled frustrated Hubbard model is commonly used to describe these materials, where pairs of organic molecules are replaced by a single effective site. We have recently demonstrated however that superconductivity is not present in this model. We are currently performing calculations including electron-electron correlations on a full monomer model for this system. Our goal is to understand the origin of the antiferromagnetic state, whether a proposed quantum spin liquid (QSL) state can occur, and how these are related to superconductivity.



Computational Material Design of Rare Earth-free Magnetic Materials

The next generation of sustainable energy applications, such as electric vehicle motors and windmill generators, demand more powerful permanent magnets. Rare-earth (RE) magnets, such as Nd-Fe-B and Sm-Co, are the strongest permanent magnets commercially available today. Although these magnets exhibit the best performance two important obstacles must be overcome for continued full utilization of these permanent magnets in sustainable energy applications. One is the low operation temperature range of these RE-based permanent magnets, and the other is the limited supply and high and unstable price of the RE metals. CCS researchers led by Prof. Seong-Gon Kim of Department of Physics and Astronomy use ab-initio computational methods to identify suitable dopants and their optimum concentration to add to base RE-free permanent magnetic materials such as Ba/Sr-hexaferrites and MnBi magnets. This research is funded by the Advanced Research Projects Agency – Energy (ARPA-E) of the Department of Energy (DOE) under the Rare Earth Alternatives for Critical Technologies (REACT) program.



Education and Outreach

CCS hosted the NSF funded Research Experiences for Undergraduates (REU) Program in Applied Mathematics and Biostatistics program led by Prof. Hyeona Lim. Several highly talented undergraduate students were selected and spent their summers on MSU campus and successfully finished research projects under the supervision of CCS faculty members. In order to disseminate new findings from our REU program, a one-day Research Experiences for Teachers (RET) workshop was also organized for Mississippi and a few other states' high school teachers in mathematical sciences.

The 9th Mississippi State-UAB Conference on Differential Equations and Computational Simulations was held on October 4-6, 2012 in McCool Hall, at MSU. With the NSF grant, graduate students and recent Ph.D.s supported for travel expenses. There were total 131 registered participants from 8 different countries. There were 10 plenary talks by the world-renowned researchers and there were also 64 contributed presentations by researchers in various disciplines working on differential equations and computational simulations.

Publications

Patents

M. J. Berg and G. Videen, "Methods and apparatus for contact-free holographic imaging of aerosol particles," (USPTO application filed March 2012, S/N: 13/423,825).

M. J. Berg, "Particle-assisted light concentration for solar photovoltaics," (USPTO provisional application filed November 2012, S/N: 61/796,112).

Peer-reviewed Journals

F. Jin, K. Michielsen, M.A. Novotny, S. Miyashita, S. Yuan, and H. De Raedt, "Quantum Decoherence Scaling with Bath Size: Importance of Dynamics, Connectivity, and Randomness," New Journal of Physics, volume 15, article 033009 [20 pages], (2013).

F. Jin, T. Neuhaus, K. Michielsen, S. Miyashita, M.A. Novotny, M.I. Katsnelson, and H. De Raedt, "Equilibration and Thermalization of Classical Systems," Physical Review A, volume 87, article 022117 [13 pages], (2013).

R. Ceolato, N. Riviere, M. J. Berg, B. Biscans, "Electromagnetic scattering from aggregates embedded in absorbing media," Progress In Electromagnetics Scattering Research (accept-ed, in press 2013).

R. Ceolato, M. J. Berg, N. Riviere, "Spectral and angular light-scattering from silica fractal aggregates," J. Quant. Spectrosc. Radiat. Transfer (accepted, in press 2013).

"Probing Flavor-Dependent EMC Ect with WBoson Production," W.-C. Chang, I. Cloet, D. Dutta and J.-C. Peng, Phys. Lett. B720, 188 (2013).

"Color transparency: Past, present and future," D. Dutta, K. Hafidi, and M. Strikman, Prog. Part. Nucl. Phys., 69,1 (2013).

Shankar P. Sastry, Jibum Kim, Suzanne M. Shontz, Brent Craven, Frank C. Lynch, Keefe B. Manning, and Thap Panitanarak, Patient-specific model generation and simulation for pre-operative surgical guidance for pulmonary embolism treatment, Invited submission to Image-Based Geometric Modeling and Mesh Generation, Springer, Lecture Notes in Computational Vision and Biomechanics, Volume 3, 223-249, 2013.

Jeonghyung Park, Suzanne M. Shontz, and Corina S. Drapaca, A combined level set/mesh warping algorithm for tracking brain and cerebrospinal fluid evolution in hydrocephalic patients, Invited submission to Image-based Modeling and Mesh Generation, Springer, Lecture Notes in Computational Vision and Biomechanics, Volume 3, 107-141, 2013.

Jibum Kim, Thap Panitanarak, and Suzanne M. Shontz, A Multiobjective Framework for Mesh Optimization, International Journal for Numerical Methods in Engineering, 94(1):20-42, March 2013.

Suzanne M. Shontz and Dragos M. Nistor, CPU-GPU algorithms for triangular surface mesh simplification, Proc. of the 2012 International Meshing Roundtable, pp. 475-492, 2013.

A.B. Misra and H. Lim, "Nonlocal Total Variation based Speckle Denoising Model", Proceedings of the Fourth International Conference on Siganal and Image Processing 2012 (ICSIP 2012) Lecture Notes in Electrical Engineering, Volume 221, 2013, pp 517-527

Wallace, L.E. and C.H. Doffitt. In press. Genetic structure of the mesic forest-adapted herbs Trillium cuneatum and Trillium stamineum (Melanthiaceae) in the south-central United States. Castanea.

Baird, R., L.E. Wallace, G. Baker, and P. Scott. In press. Stipitate Hydnums of southern United States: I: Phellodon missippiensis a new species from Mississippi. Mycotaxon.

Clay, R. T., Song, J. P., Dayal, S., & Mazumdar, S. (2012). Ground State and Finite Temperature Behavior of 1/4-filled Band Zigzag Ladders. Journal of the Physical Society of Japan. 81(7), 074707.

Dayal, S., Clay, R. T., & Mazumdar, S. (2012). Absence of Long-range Superconducting Correlations in the Frus-

trated Half-filled-band Hubbard Model. Physical Review B. American Physical Society. 85(16), 165141.

Clay, R. T., Dayal, S., Li, H., & Mazumdar, S. (2012). Beyond the Quantum Spin Liquid Concept in Frustrated Two Dimensional Organic Superconductors. Physica Status Solidi B. 249(5), 991-994.

Mazumdar, S., & Clay, R. T. (2012). Is There a Common Theme Behind the Correlated-electron Superconductivity in Organic Charge-transfer Solids, Cobaltates, Spinels and Fullerides Physica Status Solidi B. 249(5), 995-998.

Mazumdar, S., Clay, R. T., & Li, H. (2012). Similarities in Electronic Properties of Organic Charge-transfer Solids and Layered Cobaltates. Physica B. 407, 1722-1724.

M.A. Novotny, M.L. Guerra, H. De Raedt, K. Michielsen, and F. Jin, "Dynamics of a Single Spin-1/2 Coupled to x- and y-Spin Baths: Algorithm and Results," Physics Procedia, 34, (2012) 90 invited.

M.A. Novotny, M. Guerra, H. De Raedt, K. Michielsen, and F. Jin, "An Efficient Algorithm for Simulating the Real-Time Quantum Dynamics of a Single Spin-1/2 Coupled to Specific Spin-1/2 Baths," J. Physics: Conference Series, 402, (2012) 012019 [17 pages].

C. Varghese and M.A. Novotny, "Quantum Transport through Fully Connected Bethe Lattices," Inter. J. Mod. Phys. C, 23, (2012) 1240010 [10 pages] invited.

M. J. Berg, "Power-law patterns in electromagnetic scattering: A selected review and recent progress," J. Quant. Spectros. Radiat. Transfer 113 p. 2292-309 (2012) [invited review article].

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).

M. J. Berg, "Optical properties of nanoparticle systems: Mie and beyond," J. Quant. Spectros. Radiat. Transfer 113 p. 198 (2012) [invited book review].

H. Kim, V. R. Calvert, and S. Kim, Preservation of fine structures in PDE-based image de-noising. Advances in Numerical Analysis, Vol. 2012, pp. 1{19 (2012).

Y. Cha and S. Kim, The method of non at time evolution (MONTE) in PDE- based image restoration. The Journal of Korea Information and Communication Society, Vol. 11, pp. 961{971 (2012).

"New Measurements of the Transverse Beam Asymmetry for Elastic Electron Scat-tering from Selected Nuclei," S. Abrahamayan et al., Phys. Rev. Lett. 109, 192501 (2012).

"The Search for the onset of Color Transparency: a status report," D. Dutta and K. Hafidi, Int. Jour. of Mod. Phys. E21, 1230004 (2012).

"A diamond micro-strip electron detector for Compton polarimetry," A. Narayan, D. Dutta, V. Tvaskis, and J. Martin, Nuovo Cimento C035, 134 (2012).

"Amplitude analysis of n gamma n -> pi^p data above 1 GeV," W. Chen, H. Gao, W. J. Briscoe, D. Dutta, A. E. Kudryavtsev, M. Mirazita, M. W. Paris, P. Rossi, S. Stepanyan, I. I. Strakovsky, Phys. Rev. C86, 015206 (2012).

"Polarization components in pi0 photoproduction at photon energies up to 5.6 GeV," W. Luo et al., Phys. Rev. Lett. 108, 222004 (2012).

"Measurements of the neutron F2 structure function via spectator tagging with CLAS," N. Baillie et al., Phys. Rev. Lett. 108, 142001 (2012).

"Seasurement of the neutron radius of 208Pb through parity violation in electron scattering," S. Abrahamyan et al., Phys. Rev. Lett 108, 112502 (2012).

"New measurement of high-momentum nucleons and short-range structures in nuclei," N. Fomin et al., Phys Rev. Lett. 108, 092502 (2012).

"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^2 <2.7 GeV^2,”J. Huang et al., Phys Rev. Lett 108, 052001 (2012).

“Semi-inclusive charged-pion electroproduction oðrotons and deuterons: cross sections, ratios and access to quark parton model at low energies,” R. Asaturyan et al., Phys. Rev. C85, 015202 (2012).

Wheeler, G.L., M.E. McGlaughlin, and L.E. Wallace. 2012. Variable length chloroplast markers for population genetic studies in Acmispon (Fabaceae). American Journal of Botany 99:e408-e410.

Gavin S. Abo, Yang-Ki Hong, Jeevan Jalli, Jae-Jin Lee, Ji-Hoon Park, Seok Bae, Seong-Gon Kim, Byoung C. Choi, and Terumitsu Tanaka, “Shape Dependent Coercivity Simulation of a Spherical Barium Ferrite (S-BaFe) Particle with Uniaxial Anisotropy”, J. Magnetics 17, 1-5 (2012).

B. Jelinek, S. Groh, A. Moitra, M. F. Horstemeyer, J. Houze, Seong-Gon Kim, G. J. Wagner, M. I. Baskes, “MEAM potentials for the Al, Si, Mg, Cu, and Fe alloys,” Phys. Rev. B 85, 245102 [18 pages] (2012).

Laalitha Liyanage, Seong-Gon Kim, J. Houze, Sungho Kim, M. A. Tschopp, M. I. Baskes, Mark F. Horstemeyer, “Structural, elastic and thermal properties of cementite (Fe3C) calculated using Modified Embedded Atom Method,” arXiv:1202.3068 [cond-mat.mtrl-sci], under review for Phys Rev. B (2012).

Shankar Prasad Sastry, Suzanne M. Shontz, and Stephen A. Vavasis, A Log-Barrier Method for Mesh Quality Improvement and Untangling, Invited submission to Engineering with Computers; Published online before print, November 2012.

Petko Kitanov, Odile Marcotte, Wil Schilders, and Suzanne M. Shontz, A vertex cut algo-rithm for model order reduction of parasitic resistive networks, COMPEL: The Interna-tional Journal for Computation and Mathematics in Electrical and Electronic Engineering, 31(6): 1850-1871, November 2012.

Jibum Kim, Shankar Prasad Sastry, and Suzanne M. Shontz, A numerical investigation on the interplay amongst geometry, meshes, and linear algebra in the finite element so-lution of elliptic PDEs. Invited submission, Engineering with Computers, 28(4): 431-450, October 2012.

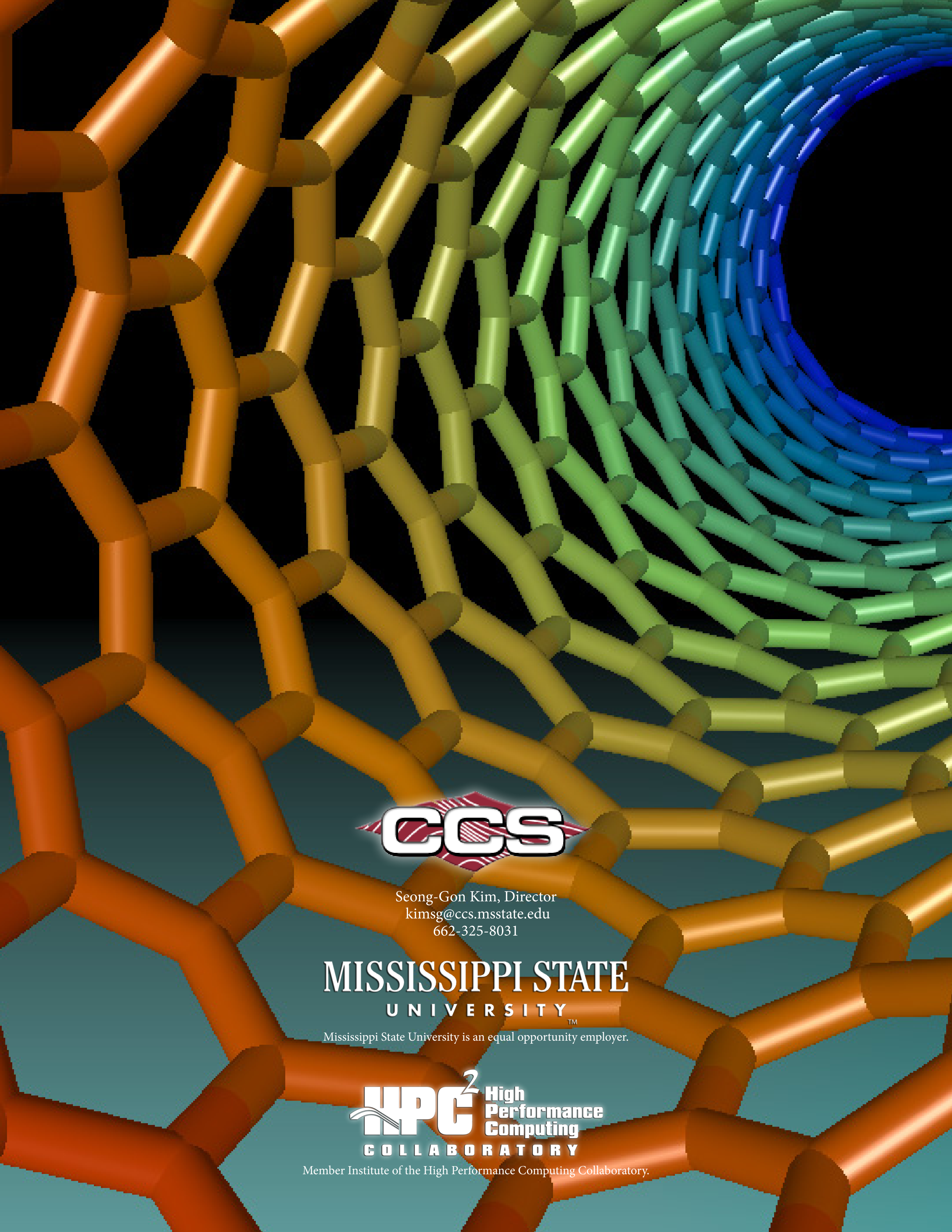
Shankar P. Sastry and Suzanne M. Shontz, Performance characterization of nonlinear optimization methods for mesh quality improvement. Invited submission, Engineering with Computers, 28(3): 269-286, 2012.

Suzanne M. Shontz and Stephen A. Vavasis, A robust solution procedure for hyperelastic solids with large boundary deformation. Engineering with Computers, 28(2): 135-147, 2012.

Jeonghyung Park, Suzanne M. Shontz, and Corina S. Drapaca, Automatic boundary evolution tracking via a combined level set method and mesh warping technique: Application to hydrocephalus, MICCAI Workshop on Mesh Processing in Medical Image Analysis 2012, Springer, Vol. 7599, p. 122-133, 2012.

Kenneth D. Czuprynski, John Fahnline, and Suzanne M. Shontz, Parallel boundary ele-ment solutions of block circulant linear systems for acoustic radiation problems with rotationally symmetric boundary surfaces, Proc. of the Internoise 2012/ASME NCAD Meeting, August 2012.

R. Damiens, H. Rhee, Y. Hwang, S.J. Park, Y. Hammi, H. Lim, and M.F. Horstemeyer, “Compressive behavior of a turtle’s shell: Experiment, modeling, and simulation,” Journal of the Mechanical Behavior of Biomedical Materials, 6 (2012) 106-112



CCS

Seong-Gon Kim, Director
kimsg@ccs.msstate.edu
662-325-8031

MISSISSIPPI STATE UNIVERSITY™

HPC² High Performance Computing COLLABORATORY

Member Institute of the High Performance Computing Collaboratory.