University of Minnesota

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25 years of supercomputing research, 1984–2009

Supercomputing Institute
for Advanced Computational Research

a unit of the Office of the Vice President for Research

Summer 2009 Research Bulletin of the Supercomputing Institute

Department of Aerospace Engineering and Mechanics

Designing Solar Vehicles

Every two years the students on the Solar Vehicle Project design, build, and race a solar car against 20 or 30 other teams from all over the world. The race is run on public roads, for over 2,000 miles. For most of those miles the car is driven at or near the race speed limit of 65 miles per hour. At that speed, drag is the dominant force on the car that must be overcome by solar power. The dominant force that tends to push the car out of its traffic lane and into danger is the side force caused by cross winds blowing across the road.

The two major design considerations for this vehicle are safety and performance. The crosswind sensitivity is a major safety consideration and the aerodynamic drag is a major performance consideration.

The students use the Ansys program at MSI to simulate the aerodynamic forces acting on the car as it races down the road, with various cross wind conditions disturbing the car. Ansys creates computational fluid dynamics simulations that take many days to run on a typical student's laptop computer. It would not be possible to make enough runs to design a safe,

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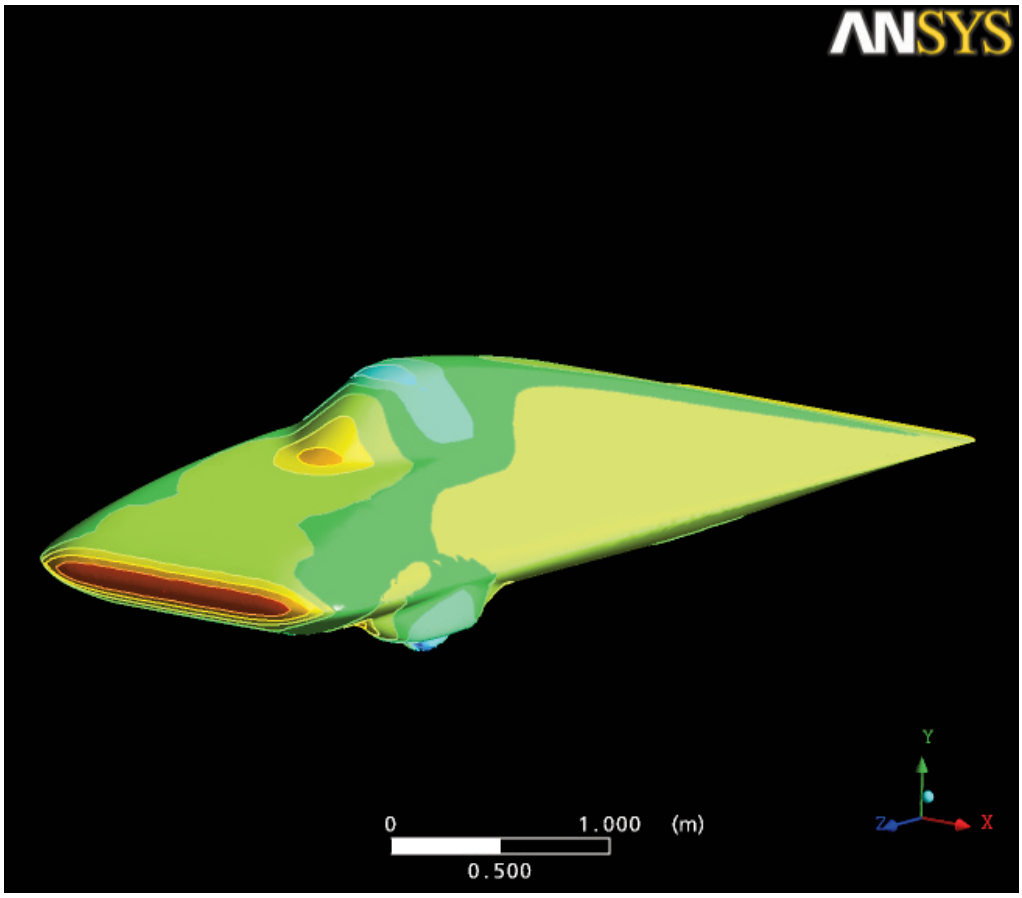


Figure 1. A contour showing the relative air pressure on the solar car. This picture shows the drop in pressure corresponding to increased airspeed over the canopy of the car.

Also in This Issue

effective car if the team had to rely on their own personal computers to do the work. The supercomputers at MSI run many cases in a few hours, giving the team an enormous capability to optimize the performance and safety of the design.

The students develop six to ten different solar car design configurations. After those car shapes are modeled in ProE (a computer-aided drafting system), the geometry is exported to software tools at MSI that create computational mesh grids that represent the shape of the car and the road surface. The grids go into the Ansys solver, which computes the airflow over and around the car. Then post-processing software at MSI calculates very accurate estimates of the lift, drag, side force, and tip-over moments caused by the airflow. The students then take that information and determine which of the various designs will have the best race performance while being safe to drive in cross wind conditions. After months of design studies and hundreds of computer simulations the design with the best performance that meets the safety requirements emerges.

The Solar Vehicle project gives the students powerful analytical skills that will serve them well in their future careers as engineers in any field, but especially in the aerospace industry. The work using MSI resources is performed by the "Aero Team" division of the solar vehicle project; these students are mostly majors in aerospace engineering and mechnics.

The solar car team has been very successful with their vehicles. The latest car, called Centaurus, won the 2009 Formula Sun Grand Prix, a closed-track race that took place in Cresson, Texas, in June 2009, completing 487 laps. This was 94 more laps than the second-place finisher. The University of Minnesota team also clocked the fastest lap, at two minutes, twenty seconds for the 1.7-mile track. The team placed fifth with Centaurus in the 2008 North American Solar Challenge race from Dallas, Texas to Calgary, Alberta, Canada.

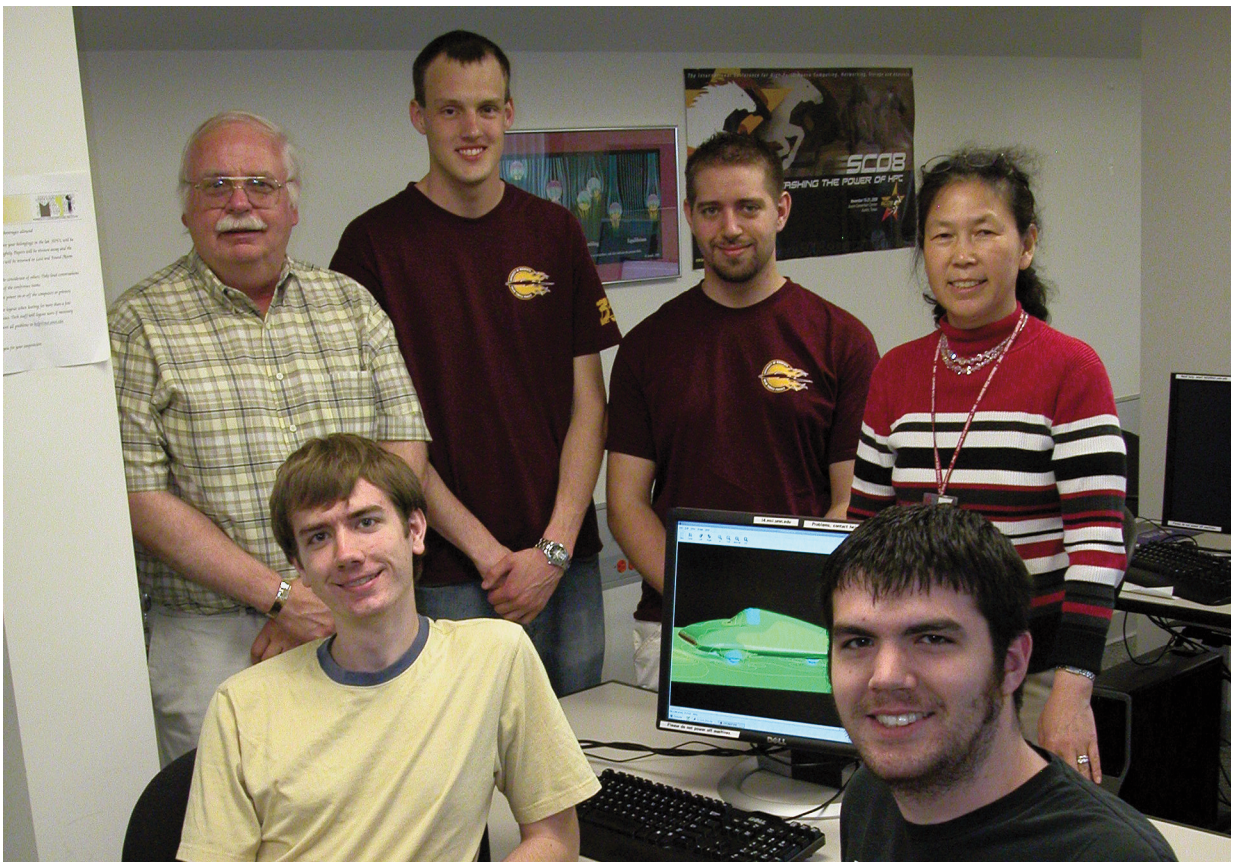


Figure 2. Standing, left to right: Dr. Jeff Hammer, Department of Aerospace Engineering and Mechanics, Solar Car Team advisor; David Towney; Peter Leonhardt; Dr. Shuxia Zhang, Supercomputing Institute. Seated, left to right: Jon Olson, Matt Higgins.

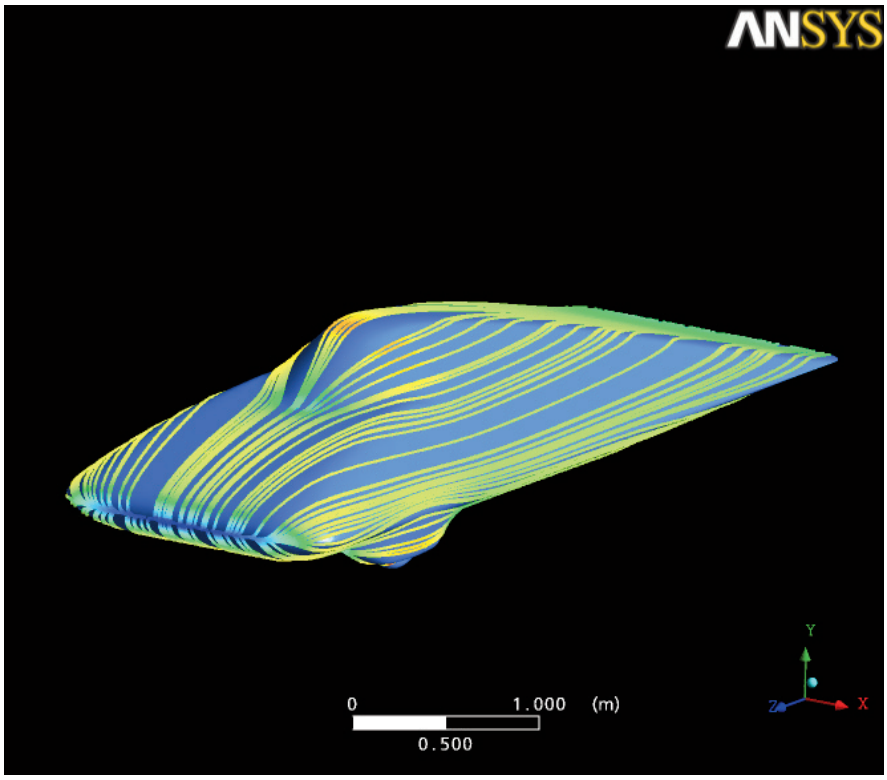
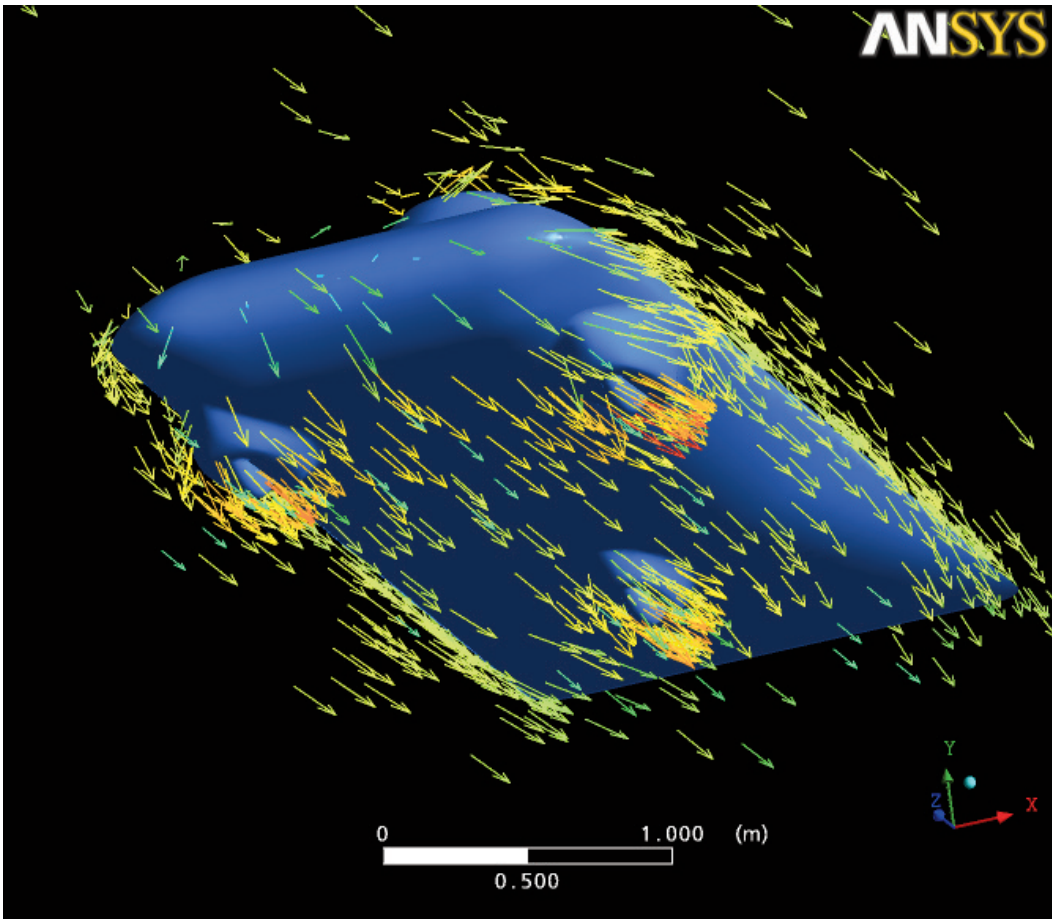


Figure 3 (left): Surface streamlines showing the path of air over the surface of the car. The color indicates airspeed, from red (high) to blue (low).

Figure 4 (below): A vector plot of the underside of the car showing flow separation at the wheels, which is minimized by adding the aerodynamic fairing around most of the wheel as shown.



Undergraduate Internship Program, Summer 2009

The Supercomputing Institute's Undergraduate Internship Program, now in its 19th year, gives undergraduates the opportunity to experience working in a research environment. The interns get to participate in a challenging and enriching educational experience that helps them decide whether they want to pursue graduate or professional education and research. Interns work with Principal Investigators at the Supercomputing Institute and their research groups on their projects. These projects can come from any of the fields represented at the Supercomputing Institute, and include all aspects of high-performance computing and scientific modeling and simulation. Interns give short presentations about their research projects and also prepare written reports.

The Summer 2009 program included 12 interns who worked on projects in a wide variety of fields. They were selected from over 80 applicants at colleges and universities in the United States and Puerto Rico. Nine of the interns worked on projects sponsored by the Supercomputing Institute's Research Experiences for Undergraduates (REU) grant from the National Science Foundation (NSF) and three were sponsored by internal MSI funds.

Bradley C. Abell, a physics major at Gustavus Adolphus College in St. Peter, Minnesota, worked with Professor J. Woods Halley, Department of Physics and Supercomputing Institute Fellow. His project was "Platinum Clusters: A Computational Study in the Search for Better Catalysts." The goal of this project was to study Pt_{13} in order to determine a way to speed up the oxygen reduction reaction in fuel cells.

Scott M. Adams, an astronomy and physics major and Chinese minor at the University of Arizona in Tucson, worked in the research group of Professor Thomas W. Jones, Department of Astronomy, Supercomputing Institute Fellow, and Interim Director of the Supercomputing Institute. Mr. Adams worked on a project called "Three-dimensional Simulations of Narrow-angle Tail Galaxies." For this project, Mr. Adams performed three-dimensional magnetohydrodynamic computer simulations of narrow-angle tail galaxies. He also processed the data to make images and movies that facilitated understanding of the results.

Professor David A. Yuen, Department of Geology and Geophysics and Supercomputing Institute Fellow, hosted two interns this year. **Gregory A. Barnett** is an applied mathematics major at Boise State University in Idaho, and **Robin M. Weiss** is a computer science major at Macalester College in St. Paul, Minnesota. Mr. Barnett's project was called "High Rayleigh Number, 3-D Mantle Convection With Standard and Compact Finite Difference Methods Implemented on the GPU." He developed algorithms for simulating three-dimensional mantle convection. Mr. Weiss worked on a project called "Web-based Interactive Visualization in

Above: Interns, faculty advisors, research group members, and MSI staff enjoy the Intern Program Welcome Reception.

Above, left to right: Adam Birdsall, Bradley Abell, Erik Fritz, Aurora Turgeon, Erik Gustafson, Jacob Stricherz, Scott Adams, Abhrajeet Roy, and Yi Wang.

Real Time," which investigated the use of the World Wide Web for interactive computing. These projects are part of Professor's Yuen's ongoing work concerning mantle convection and interactive supercomputing, which was featured in the Summer 2007 issue of the *Research Bulletin*.

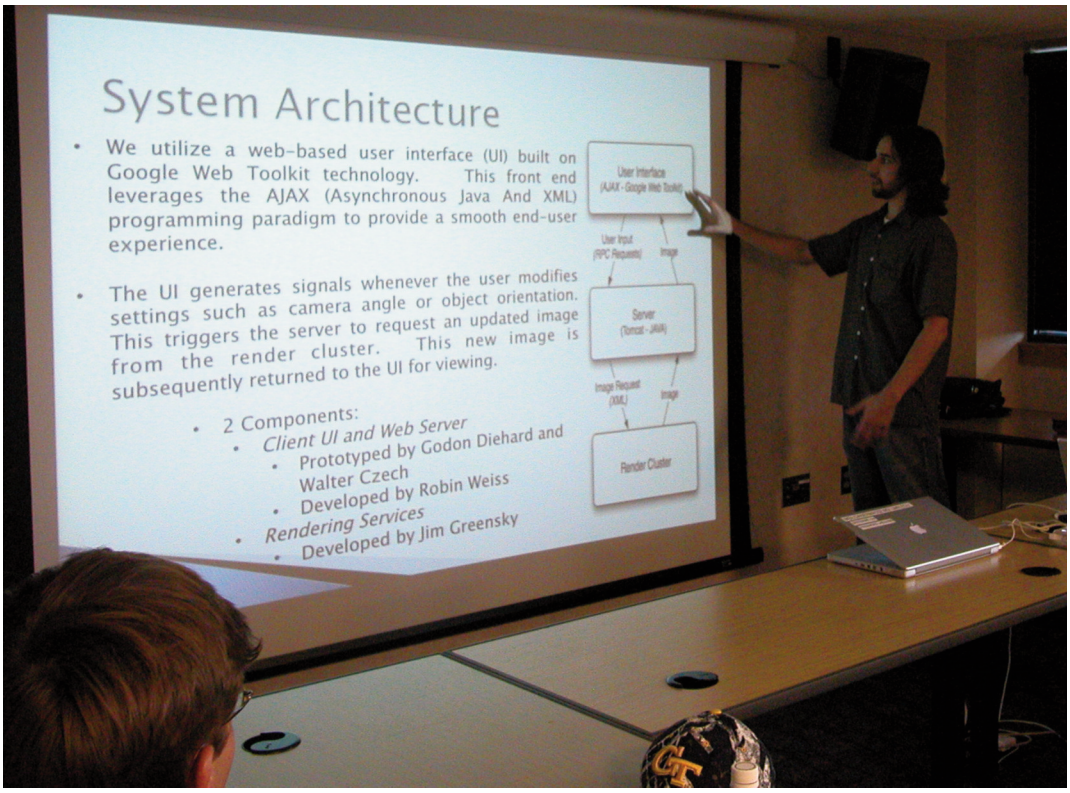
Adam W. Birdsall, from Oberlin College in Ohio, is a chemistry and piano double major with a minor in mathematics. He worked with Associate Professor William B. Gleason, Department of Laboratory Medicine and Pathology and Supercomputing Institute Fellow, on a project titled "Comparative Docking Studies of Gleevec." Mr. Birdsall compared docking programs to find the one best suited to the Gleason group's research, and gained insights about docking by working with the small molecule Gleevec.

University of Minnesota chemistry major **Erik M. Fritz** worked with Professor Steven A. Kass, Department of Chemistry and Supercomputing Institute Associate Fellow. His project was "Determining Relative Acidities in Carboxylic Acids." For this project, Mr. Fritz used the programs Spartan08 and Gaussian03 to compute the energies of different molecules so their gas-phase acidities could be calculated.

Two interns worked this summer with the group of Assistant Professor Elizabeth A. Amin, Department of Medicinal Chemistry. **Erik R. Gustafson** attends the Georgia Institute of Technology in Atlanta, Georgia as a biomedical engineering major with an organic/biochemistry minor, and **Abhrajeet V. Roy** is a bioengineering major/neuroscience minor at the University of Pennsylvania in Philadelphia. Mr. Gustafson's project was called "Structure-based Design and Optimization of Anthrax Toxin Lethal Factor Inhibitor." Mr. Roy, who was also an intern with Professor Amin last summer, worked on a project called "Applying Pharmacophore Mapping and Genetic Algorithms Towards the Development of Novel Anthrax Lethal Factor Inhibitors." Mr. Roy studied chemical compounds that might potentially inhibit the Anthrax Lethal Factor (ALF), and Mr. Gustafson tried to optimize identified compounds for ALF inhibition. These projects are part of research by the Amin group that was featured in the Spring 2009 *Research Bulletin*.

University of Minnesota chemical engineering and chemistry major **Sarah E. Kragt** worked with the research group of Regents Professor Donald G. Truhlar, Department of Chemistry and Supercomputing Institute Fellow. Ms. Kragt worked on a project called "Solvation Energies of Biomedical Molecules." She tested the accuracy of the SMx solvation series on large molecules as part of ongoing research in the Truhlar group.

Jacob L. Stricherz, a Universi-



Above: Intern Robin Weiss gives his final presentation.

ty of Minnesota biology major, worked with Dr. Yuk Sham, Assistant Director of the Center for Drug Design. Mr. Stricherz worked on "A Study of Beta Lactamase Inhibitors." He studied the mode of binding in beta-lactam antibiotics and beta-lactamase inhibitors in the serine beta-lactamase protein TEM-1.

Aurora J. Turgeon, who attends the University of Minnesota Morris as a chemistry major and mathematics minor, worked with Professor Christopher J. Cramer, Department of Chemistry and MSI Fellow. Her project was entitled, "^{15}N and ^{13}C Isotope Effects of Substituted Anilines." The objective of this project was to computationally support the observed ^{15}N and ^{13}C isotope effects for various substituted anilines.

University of Minnesota chemistry major **Yi Z. Wang** worked with Professor David D. Thomas, Department of Biochemistry, Molecular Biology, and Biophysics and MSI Fellow. Mr. Wang's project was called "Molecular Dynamic Simulation of TOAC Amino Acid Spin Label." The goal of this project was to understand the motion of TOAC acid spin label.

MSI will hold another Undergraduate Internship Program in Summer 2010. Projects, application instructions, and other information about the 2010 program will be posted on the MSI website (*www.msi.umn.edu*) in Fall 2009.

Bioinformatics: Building Bridges 2009

Bioinformatics: Building Bridges, the symposium of bioinformatics at the University of Minnesota, was held at the University's Walter Library on April 16–17, 2009. The symposium included participants from academics, industry, and non-profit institutions. The first day of the symposium was dedicated to tutorials (see sidebar, below) and a talk by Dr. Pascal Braun, senior scientist at the Center for Cancer Systems Biology at the Dana Farber Cancer Institute at Harvard University. This talk, "Binary Interactome Mapping to Study Human Disease," was co-sponsored by the Consortium for Bioinformatics and Computational Biology. The second day of the symposium included a poster session and six talks (see sidebars on pages 8 and 9 for poster and presentation titles). Information about the Graduate Minor in Bioinformatics at the University of Minnesota and about Computational Biology and Bioinformatics at MSI was also exhibited during the symposium.

Sponsors for the symposium included: the Graduate Program in Bioinformatics; the Graduate Program in Health Informatics; the Digital Technology Center; the Minnesota Supercomputing Institute; the Institute of Technology; the Consortium for Bioinformatics and Computational Biology; the College of Food, Agricultural, and Natural Resource Sciences; the College of Biological Sciences; the Academic Health Center; and IBM. The Program Committee was Professor Lynda B. Ellis (Department of Biochemistry, Molecular Biology, and Biophysics and Supercomputing Institute Associate Fellow), Assistant Professor Chad L. Myers (Department of Computer Science and Engineering), and Professor Nevin Dale Young (Department of Plant Pathology and Supercomputing Institute Associate Fellow).

Poster and exhibit abstracts, speaker information, and other information about this symposium can be found at:

www.binf.umn.edu/bisymp09/

Tutorials

Bioinformatics Programming
Zheng Jin Tu, Supercomputing Institute

Microarray Technology and Software Tools
Wayne Xu, Supercomputing Institute

Introduction to Similarity Searching Using BLAST
Carlso Sosa, IBM

Zheng Jin Tu, Supercomputing Institute

Running R/S-PLUS Applications at MSI - Getting Started With R and S-PLUS
Haoyu Yu, Supercomputing Institute

Proteomics Software Available in the Public Domain
Pratik Jagtap, Supercomputing Institute

Literature Resources for Bioinformatics
Peter Kirlew, University Libraries

Presentations

Analysis Methods in Mass-Spectrometry-Based Proteomics
Frank Suits, IBM

The Biomedical Informatics and Computational Biology Graduate Program
John Carlis, Department of Computer Science and Engineering

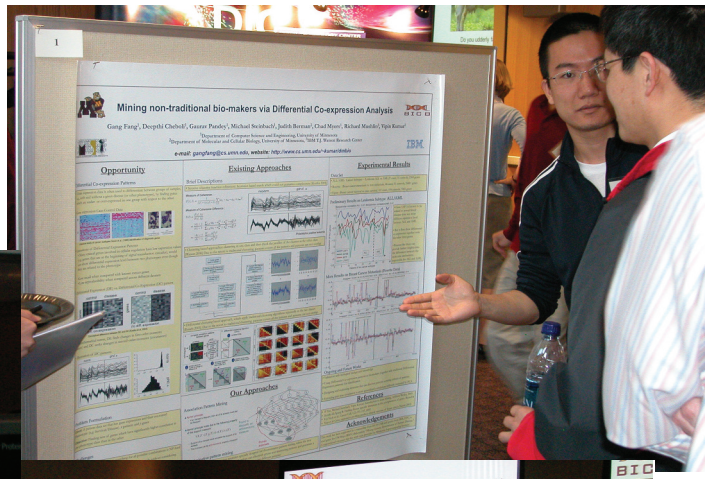
High-Resolution Mapping of Multi-Chromosome DNA Copy Number Variations in Autism
Scott Selleck, Department of Genetics, Cell Biology, and Development
Ahmed Tewfik, Department of Electrical and Computer Engineering

Toward Global Quantitative Characterization of the Yeast Genetic Interaction Network
Chad Myers, Department of Computer Science and Engineering

Unraveling Genomes and Transcriptomes Using Next Generation Sequencing
Joann Mudge, National Center for Genome Resources

Mining the Medicago Genome: A Model for Legumes and Symbiosis
Nevin Dale Young, Department of Plant Pathology

Clockwise from right: Graduate student Gang Fang explains his group's poster; Professor John Carlis (University of Minnesota) begins his presentation; Professor Nevin Dale Young (University of Minnesota) talks with Dr. Joanne Mudge (National Center for Genome Resources)



Posters

Efficient Discriminative Patterns Mining From Dense and High Dimensional Biomedical Data
Gang Fang, Deepthi Cheboli, Gaurav Pandy, Michael Steinbach, and Vipin Kumar
Department of Computer Science and Engineering

Computational Alanine Scanning of the Alpha-lactamase Inhibitor Protein and TEM-1 Alpha-lactamase Complex
Hiqmet Kamberaj and Yuk Sham
Center for Drug Design

Improving Biodegradation Pathway Prediction
Jungeng Gao[1], Larry P. Wackett[2], and Lynda B.M. Ellis[1]
[1]Institute for Health Informatics
[2]Department of Biochemistry, Molecular Biology, and Biophysics

Divergence and Redundancy Among Duplicate Genes in S. Cerevisiae
Jeremy Bellay and Benjamin VanderSluis
Department of Computer Science and Engineering

Identification of Molecular Targets of the RNA-binding Protein CUGBP1 Through Computational Sequence Analysis
Daneil Beisan, Bernd Rattenbacher, Paul Bohjanen, and Irina Vlasova
Center for Infectious Diseases and Microbiology Translational Research, Department of Microbiology

Automated Identification of Idiosyncratic Drug-Induced Liver Injury
Gowtham Atluri[1], Rohit Gupta[1], Michael Steinbach[1], Vipin Kumar[1], Piet de Groen[2]
[1]Department of Computer Science and Engineering
[2]Gastroenterology, Mayo Clinic

Colon Cancer not Prevented by Colonoscopy
Rohit Gupta[1], Michael Steinbach[1], Vipin Kumar[1], Piet de Groen[2]
[1]Department of Computer Science and Engineering
[2]Gastroenterology, Mayo Clinic

Association Analysis-based Extraction of Functional Information From Genomic Data
Gaurav Pandy, Gowtham Atluri, Michael Steinbach, Rohit Gupta, Tushar Garg, and Vipin Kumar
Department of Computer Science and Engineering

Data Mining for Connecting SNPs and Disease
Rohit Gupta[1], Gang Fang[1], Gowtham Atluri[1], Michael Steinbach[1], Brian Van Ness[2], and Vipin Kumar[1]
[1]Department of Computer Science and Engineering
[2]Department of Genetics, Cell Biology, and Development

MSI Seed Grants for 2009–2010

The MSI Seed Grant program has awarded four grants for the academic year 2009–2010. The Seed Grant program supports new efforts that advance the level of high-performance computational research at the University of Minnesota and that stand to significantly incorporate MSI resources and enhance its impact. The specific objective is to encourage development of research initiatives that will increase the local, national, and international impact and visibility of the University in the high-performance computational research arena.

Abstracts for the Seed Grant projects can be found at our website:

www.msi.umn.edu/programs/seedgrant.html

Seed Grant Projects, 2009–2010

Color Appearance Modeling for Physics-based Coatings
PI: Gary W. Meyer, Department of Computer Science and Engineering

Machine Learning Approaches for Inference of Genetic Interaction Networks in Yeast
PI: Chad L. Myers, Department of Computer Science and Engineering

A High-Performance Large-eddy Simulation Technique to Study Land-Atmosphere Fluxes Over Multiscale Topography
PI: Fernando Porté-Agel, Department of Civil Engineering, St. Anthony Falls Laboratory, and MSI Fellow

Highly Scalable Particle Simulation for Multiscale Gas Flows
PI: Thomas E. Schwartzentruber, Department of Aerospace Engineering and Mechanics

MSI Open House

The Supercomputing Institute will host an Open House on Wednesday, November 4, 2009. Attendees will be able to tour our facilities, including the machine room, the Scientific Development and Visualization Lab, and the LCSE-MSI Visualization Lab. They will also be able to see demonstrations of software available at MSI and displays about current research being performed at MSI. There will also be food, goody bags, and door prizes.

The Open House will held on November 4, 11:30–3:30, in the MSI facilities on the fourth and fifth floors of Walter Library. Walter is located on the Mall on the East Bank campus. Information about the Open House will be posted on the MSI website as it becomes available:

www.msi.umn.edu

In Memoriam: H. Ted Davis

Regents Professor H. Ted Davis, Department of Chemical Engineering, passed away on May 17, 2009. Professor Davis was also Director of the BioTechnology Institute, and formerly held the positions of Dean of the Institute of Technology and Head of the Department of Chemical Engineering.

Professor Davis had been a Principal Investigator and MSI Fellow since the very early days of the Institute. His recent research at MSI involved several areas, including using particle-based simulation techniques to study the dynamics and rheology of complex fluids, using molecular dynamics and Monte Carlo simulation techniques to investigate diblock copolymers in epoxy, and studying the computational aspects of continuum and network theories of fluid physics and transport.

The staff of the Institute express their deepest condolences to Professor Davis's family, friends, and colleagues.

Aerospace Engineering and Mechanics

2009/33
Efficient Algorithms for Discrete Lattice Calculations
M. Arndt, V. Sorkin, and **E.B. Tadmor**

Biochemistry, Molecular Biology, and Biophysics

2009/55 and CB 2009-21
On the Function of Pentameric Phospholamban: Ion Channel or Storage Form?
L. Becucci, A. Cembran, C.B. Karim, **D.D. Thomas**, R. Guidelli, **J. Gao**, and **G. Veglia**

Cancer Center

2009/20 and CB 2009-11
A Conditional Transposon-based Insertional Mutagenesis Screen for Genes Associated With Mouse Hepatocellular Carcinoma
V.W. Keng, A. Villanueva, D.Y. Chiang, A.J. Dupuy, B.J. Ryan, I. Matise, **K.A.T. Silverstein**, A. Sarver, T.K. Starr, K. Akagi, L. Tessarollo, L.S. Collier, S. Powers, S.W. Lowe, N.A. Jenkins, N.G. Copeland, J.M. Llovet, and **D.A. Largaespada**

2009/21 and CB 2009-12
A Transposon-based Genetic Screen in Mice Identifies Genes Altered in Colorectal Cancer
T.K. Starr, R. Allaei, **K.A.T. Silverstein**, R.A. Staggs, A.L. Sarver, T.L. Bergemann, M. Gupta, M.G. O'Sullivan, I. Matise, A.J. Dupuy, L.S. Collier, S. Powers, A.L. Oberg, Y.W. Asmann, S.N. Thibodeau, L. Tessarollo, N.G. Copeland, N.A. Jenkins, R.T. Cormier, and **D.A. Largaespada**

Center for Drug Design

2009/76 and CB 2009-30
Selective Inhibition of Nicotinamide Adenine Dinucleotide Kinases by Dinucleoside Disulfide Mimics of Nicotinamide Adenine Dinucleotide Analogues
R. Petrelli, **Y.Y. Sham**, L. Chen, K. Felczak, E. Bennett, D. Wilson, **C. Aldrich**, J.S. Yu, L. Cappellacci, P. Franchetti, M. Grifantini, F. Mazzola, M. Di Stefano, G. Magni, and K.W. Pankiewicz

Chemical Engineering (UMD)

2009/18
Effects of Incompressible Surfactant on Thermocapillary Interactions of Spherical Drops
M.A. Rother

Chemical Engineering and Materials Science

2009/25 and CB 2009-13
Coupled Flow and Reaction During Natural Convection PCR
J.W. Allen, M. Kenward, and **K.D. Dorfman**

2009/26 2009
A Schur Complement Formulation for Solving Free-boundary, Stefan Problems in Solidification
L. Lun, A. Yeckel, and **J.J. Derby**

2009/66
Viscosity Hills in the Lower Mantle: Influence From the Iron High-to-Low Spin Transition
J.F. Justo, Z.Q. Wu, **D.A. Yuen**, and **R.M. Wentzcovitch**

2009/70
Modeling the Crystal Growth of Cadmium Zinc Telluride: Accomplishments and Future Challenges
J.J. Derby, D. Gasperino, N. Zhang, and A. Yeckel

2009/71
Effect of Site Degeneracies on the Spin Crossovers in (Mg,Fe)SiO_3 Perovskite
K. Umemoto, H. Hsu, and **R.M. Wentzcovitch**

2009/72
Quantum Espresso: A Modular and Open-Source Software Project for Quantum Simulations of Materials
P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. de Gironcoli, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin Samos Colomer, N. Marzari, F. Mauri, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A.P. Seitsonen, A. Smogunov, P. Umari, and **R.M. Wentzcovitch**

Chemistry

2009/12
Gas-Phase Versus Liquid-phase Structures by Electrospray Ionization Mass Spectrometry
Z. Tian and **S.R. Kass**

2009/19 and CB 2009-10
Unraveling the Mechanisms of Ribozyme Catalysis With Multi-Scale Simulations
T.-S. Lee, G.M. Giambasu, A. Moser, K. Nam, C. Silva-Lopez, F. Guerra, O. Nieto-Faza, T.J. Giese, and **D.M. York**

2009/27 and CB 2009-14
Are Carboxyl Groups the Most Acidic Sites in Amino Acids? Gas-Phase Acidities, Photoelectron Spectra, and Computations on Tyrosine, p-Hydroxybenzoic Acid, and Their Conjugate Bases
Z. Tian, X.-B. Wang, L.-S. Wang, and **S.R. Kass**

Names of Supercomputing Institute principal investigators appear in bold type. This list contains reports entered into the reports database during April–July 2009.

2009/28
Gas-Phase Synthesis and Reactivity of the Lithium Acetate Enolate Anion, $-CH_2CO_2Li$
M.M. Meyer, G.N. Khairallah, **S.R. Kass**, and R.A.J. O'Hair

2009/36 and CB 2009-15
X-Pol Potential: An Electronic Structure-based Force Field for Molecular Dynamics Simulation of a Solvated Protein in Water
W. Xie, M. Orozco, **D.G. Truhlar**, and **J. Gao**

2009/37
A Study of the Ground and Excited States of Al_3 and Al_3–. II. Computational Analysis of the 488 nm Anion Photoelectron Spectrum and a Reconsideration of the Al_3 Bond Dissociation Energy
S.R. Miller, N.E. Schultz, **D.G. Truhlar**, and **D.G. Leopold**

2009/39
Mechanistic Analysis of the Base-catalyzed HF Elimination From 4-Fluoro-4-(4´-nitrophenyl)butane-2-one Based on Liquid-phase Kinetic Isotope Effects Calculated by Dynamics Modeling With Multidimensional Tunneling
Y. Kim, A.V. Marenich, J. Zheng, K.H. Kim, M. Koodziejska-Huben, M. Rostkowski, P. Paneth, and **D.G. Truhlar**

2009/40
Benchmark Energetic Data in a Model System for Grubbs II Metathesis Catalysis and Their Use for the Development, Assessment, and Validation of Electronic Structure Methods
Y. Zhao and **D.G. Truhlar**

2009/41
Bond Angle Distributions of Carbon Dioxide in the Gas, Supercritical, and Solid Phases
K.E. Anderson, S.L. Mielke, **J.I. Siepmann**, and **D.G. Truhlar**

2009/42
Efficient Global Representations of Potential Energy Functions: Trajectory Calculations of Bimolecular Gas-phase Reactions by Multiconfiguration Molecular Mechanics
O. Tishchenko and **D.G. Truhlar**

2009/43 and CB 2009-16
Performance of SM6, SM8, and SMD on the SAMPL1 Test Set for the Prediction of Small-molecule Solvation Free Energies
A.V. Marenich, **C.J. Cramer**, and **D.G. Truhlar**

2009/44 and CB 2009-17
Critical Role of Substrate Conformational Change in the Proton Transfer Process Catalyzed by 4-Oxalocrotonate Tautomerase
J.J. Ruiz-Pernia, M. Garcia-Viloca, S. Bhattacharyya, **J. Gao**, **D.G. Truhlar**, and I. Tunon

2009/45
Valence–Bond Order (VBO): A New Approach to Modeling Reactive Potential Energy Surfaces for Complex Systems, Materials, and Nanoparticles
M. Zhao, M.A. Iron, P. Staszewski, N.E. Schultz, R. Valero, and **D.G. Truhlar**

2009/46 and CB 2009-18
Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions
A.V. Marenich, **C.J. Cramer**, and **D.G. Truhlar**

2009/47
Reply to Comment on "A Universal Approach to Solvation Modeling"
C.J. Cramer and **D.G. Truhlar**

2009/48
Calculation of Semiconductor Band Gaps With the M06-L Density Functional
Y. Zhao and **D.G. Truhlar**

2009/54 and CB 2009-20
Tilt and Azimuthal Angles of a Transmembrane Peptide: A Comparison Between Molecular Dynamics Calculations and Solid-State NMR Data of Sarcolipin in Lipid Membranes
L. Shi, A. Cembran, **J. Gao**, and **G. Veglia**

2009/55 and CB 2009-21
On the Function of Pentameric Phospholamban: Ion Channel or Storage Form?
L. Becucci, A. Cembran, C.B. Karim, **D.D. Thomas**, R. Guidelli, **J. Gao**, and **G. Veglia**

2009/56
An Effective Hamiltonian Molecular Orbital-Valence Bond (MOVB) Approach for Chemical Reactions as Applied to the Nucleophilic Substitution Reaction of Hydrosulfide Ion and Chloromethane
L. Song, Y. Mo, and **J. Gao**

2009/57 and CB 2009-22
Determination of the Structure Form of the Fourth Ligand of Zinc in Acutolysin A Using Combined Quantum Mechanical and Molecular Mechanical Simulation
E.L. Wu, K.-Y. Wong, X. Zhang, K. Han, and **J. Gao**

2009/60 and CB 2009-25
Energies, Geometries, and Charge Distributions of Zn Molecules, Clusters, and Biocenters From Coupled Cluster, Density Functional, and Neglect of Diatomic Differential Overlap Models
A. Sorkin, **D.G. Truhlar**, and **E.A. Amin**

2009/61 and CB 2009-26
Perspective on Diabatic Models of Chemical Reactivity as Illustrated by the Gas-phase SN2 Reaction of Acetate Ion With 1,2-Dichloroethane
R. Valero, L. Song, **J. Gao**, and **D.G. Truhlar**

2009/62 and CB 2009-27
A Coupled Polarization-matrix Inversion and Iteration Approach for Accelerating the Dipole Convergence in a Polarizable Potential Function
W. Xie, J. Pu, and **J. Gao**

2009/73
The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights
J. Zheng, Y. Zhao, and **D.G. Truhlar**

2009/74
Efficient Diffuse Basis Sets: cc-pVxZ+ and maug-cc-pVxZ
E. Papajak, H.R. Leverentz, J. Zheng, and **D.G. Truhlar**

2009/75 and CB 2009-29
Quantum Catalysis in Enzymes
A. Dybala-Defratyka, P. Paneth, and **D.G. Truhlar**

Chemistry and Biochemistry (Duluth)

2009/65
Driven On- and Off-lattice Gas
P.D. Siders

Civil Engineering

2009/23
Modeling Wheel-induced Rutting in Soils: Rolling
J.P. Hambleton and **A. Drescher**

2009/24
Asymptotics in Soil-Wheel Interaction
J.P. Hambleton and **A. Drescher**

2009/32
Transient Heat Conduction in a Medium With Multiple Spherical Cavities
E. Gordeliy, **S.L. Crouch**, and S.G. Mogilevskaya

2009/67 and CB 2009-28
Numerical Investigation of the Hydrodynamics of Anguilliform Swimming in the Transitional and Inertial Flow Regimes
I. Borazjani and **F. Sotiropoulos**

2009/68
Vortex-induced Vibrations of Two Cylinders in Tandem Arrangement in the Proximity–Wake Interference Region
I. Borazjani and **F. Sotiropoulos**

2009/69
Detached Eddy Simulation of Flow Around Two Wall-mounted Cubes in Tandem
J. Paik, **F. Sotiropoulos**, and **F. Porté-Agel**

Computer Science and Engineering

2009/29
Hypergraph Partitioning for Sparse Linear Systems: A Case Study With a Simple Discontinuous PDE
M. Sosonkina and **Y. Saad**

2009/30
Preconditioning Helmholtz Linear Systems
D. Osei-Kuffuor and **Y. Saad**

2009/31
Trace Optimization and Eigenproblems in Dimension Reduction Methods
E. Kokiopoulou, J. Chen, and **Y. Saad**

Economics

2009/22
The Role of Labor and Marriage Markets, Preference Heterogeneity and the Welfare System in the Life Cycle Decisions of Black, Hispanic and White Women
P. Bajari

Environmental Health Sciences

2009/35
A New Semivolatile Aerosol Dichotomous Sampler
S. Won Kim and **P.C. Raynor**

Genetics, Cell Biology, and Development

2009/20 and CB 2009-11
A Conditional Transposon-based Insertional Mutagenesis Screen for Genes Associated With Mouse Hepatocellular Carcinoma
V.W. Keng, A. Villanueva, D.Y. Chiang, A.J. Dupuy, B.J. Ryan, I. Matise, **K.A.T. Silverstein**, A. Sarver, T.K. Starr, K. Akagi, L. Tessarollo, L.S. Collier, S. Powers, S.W. Lowe, N.A. Jenkins, N.G. Copeland, J.M. Llovet, and **D.A. Largaespada**

2009/21 and CB 2009-12
A Transposon-based Genetic Screen in Mice Identifies Genes Altered in Colorectal Cancer
T.K. Starr, R. Allaei, **K.A.T. Silverstein**, R.A. Staggs, A.L. Sarver, T.L. Bergemann, M. Gupta, M.G. O'Sullivan, I. Matise, A.J. Dupuy, L.S. Collier, S. Powers, A.L. Oberg, Y.W. Asmann, S.N. Thibodeau, L. Tessarollo, N.G. Copeland, N.A. Jenkins, R.T. Cormier, and **D.A. Largaespada**

Geology and Geophysics

2009/16 and CB 2009-8
Detecting Clusters of Microcalcifications in High-resolution Mammograms Using Support Vector Machines
K. Boryczko, M. Kurdziel, and **D.A. Yuen**

2009/49 and CB 2009-19
A 3-D Model of Tumor Progression Based on Complex Automata Driven by Particle Dynamics
R. Wcislo, W. Dzwinel, **D.A. Yuen**, and A.Z. Dudek

2009/50
3-D Dynamics of Hydrous Thermal-Chemical Plumes in Oceanic Subduction Zones
G. Zhu, T. Gerya, **D.A. Yuen**, S. Honda, T. Yoshida, and J.A.D. Connolly

2009/51
Small-scale Thermal and Thermo-Chemical Convection Modelling in the Lowermost Mantle and Seismic Expression of Post-perovskite Phase Transitions From Multi-scale Analysis
A.P. van den Berg, M.V. De Hoop, **D.A. Yuen**, A. Duchkov, R.D. van der Hilst, and M.H.G. Jacobs

2009/52
The Fate of the Slabs Interacting With a Viscosity Hill in the Mid-mantle
G. Morra, **D.A. Yuen**, L. Boschi, P. Chatelain, P. Koumoutsakos, and P.J. Tackley

2009/53
Seismic Imaging of the D" and Constraints on the Core Heat Flux
M. Monnereau and **D.A. Yuen**

2009/63
Time-dependent, Irreversible Entropy Production and Geodynamics
K. Regenauer-Lieb, A. Karrech, H.T. Chua, F.G. Horowitz, and **D.A. Yuen**

2009/64
Numerical Evaluation of Tsunami Wave Hazards in Harbors Along the South China Sea
H.H. Jing, H. Zhang, **D.A. Yuen**, and Y. Shi

2009/66
Viscosity Hills in the Lower Mantle: Influence From the Iron High-to-Low Spin Transition
J.F. Justo, Z.Q. Wu, **D.A. Yuen**, and **R.M. Wentzcovitch**

Institute for Therapeutics Discovery and Development

2009/59 and CB 2009-24
Total Synthesis and Evaluation of 22-(3-azidobenzoyloxy)methyl epothilone C for Photoaffinity Labeling of β-tubulin
O.E. Hutt, J. Inagaki, B.S. Reddy, S.K. Nair, E.A. Reiff, J.T. Henri, J.F. Greiner, D.G. VanderVelde, T.-L. Chiu, **E.A. Amin**, R.H. Himes, and **G.I. Georg**

Mechanical Engineering

2009/34
Coagulation of Nanoparticles in a Plasma
L. Ravi and **S.L. Girshick**

Medicinal Chemistry

2009/59 and CB 2009-24
Total Synthesis and Evaluation of 22-(3-azidobenzoyloxy)methyl epothilone C for Photoaffinity Labeling of β-tubulin
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2009/60 and CB 2009-25
Energies, Geometries, and Charge Distributions of Zn Molecules, Clusters, and Biocenters From Coupled Cluster, Density Functional, and Neglect of Diatomic Differential Overlap Models
A. Sorkin, **D.G. Truhlar**, and **E.A. Amin**

Otolaryngology

2009/58 and CB 2009-23
Parallelization of Training of a Neural Network
V. Pandit

Physical Medicine and Rehabilitation

2009/17 and CB 2009-9
Effect of Cardiogenic Pulmonary Edema on Defibrillation Efficacy
F. Yang and **R.P. Patterson**

Plant Biology

2009/20 and CB 2009-11
A Conditional Transposon-based Insertional Mutagenesis Screen for Genes Associated With Mouse Hepatocellular Carcinoma
V.W. Keng, A. Villanueva, D.Y. Chiang, A.J. Dupuy, B.J. Ryan, I. Matise, **K.A.T. Silverstein**, A. Sarver, T.K. Starr, K. Akagi, L. Tessarollo, L.S. Collier, S. Powers, S.W. Lowe, N.A. Jenkins, N.G. Copeland, J.M. Llovet, and **D.A. Largaespada**

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Urologic Surgery

2009/13 and CB 2009-5
Realistic Soft Tissue Deformation Strategies for Real Time Surgery Simulation
Y. Shen, X. Zhou, N. Zhang, **K. Tamma**, and **R. Sweet**

2009/14 and CB 2009-6
The Family of Optimal Time Integration Algorithms for Real Time Virtual Surgery
X. Zhou, Y. Shen, N. Zhang, D. Sha, **K.K. Tamma**, and **R. Sweet**

2009/15 and CB 2009-7
Interactive Collision Response Solutions to Interpenetration Problems Among Tissues and Instruments in Virtual Laparoscopic Surgery
Y. Shen, X. Zhou, N. Zhang, D. Sha, **K. Tamma**, and **R. Sweet**

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