Medical Devices

Medical Device Invention and Evaluation Through Simulation, Visualization, and Interactive Design

Rapid advances in high-performance (supercomputing) simulations are revolutionizing biomedicine in both the research and industrial context. Scientists and engineers now run patient-specific computational fluid dynamics (CFD) and finite element analysis (FEA) simulations at unprecedented levels of resolution and accuracy. A driving force behind these advances is growing interest on the part of both industry and the Food and Drug Administration (FDA) in using computer modeling and simulation to support medical device innovation and validation. As new capabilities to better incorporate simulation into engineering practice emerge, these can have a transformative impact on medical device engineering and medicine. For example, a medical device designer could have access to early, accurate feedback on device performance and be able to exhaustively explore many design iterations. In this way, simulation could reduce the time it takes to reach bench tests and animal trials, make these trials more efficient and effective, and, in time, overtake these methods as the primary evaluative approach in device design. To realize this potential will require tackling several difficult research challenges.

A group of University of Minnesota researchers have begun a collaboration to work toward a vision of an immersive design environment composed of coupled components for running simula-
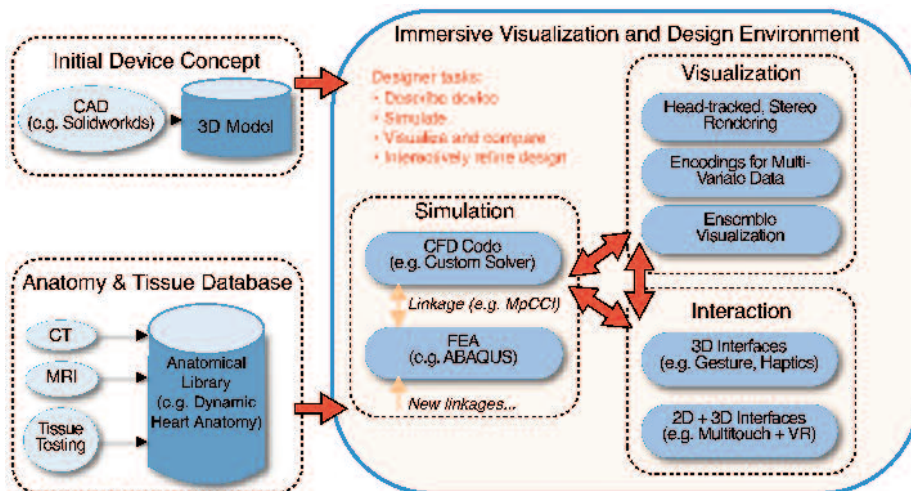

Figure 1. A new data-intensive medical device design workflow is made possible by rapidly advances in high-performance supercomputing. The system design shown here couples simulation, visualization, and interaction with the goal of improving early design feedback and evaluation and, eventually, leading to improved design of safe and effective medical devices.
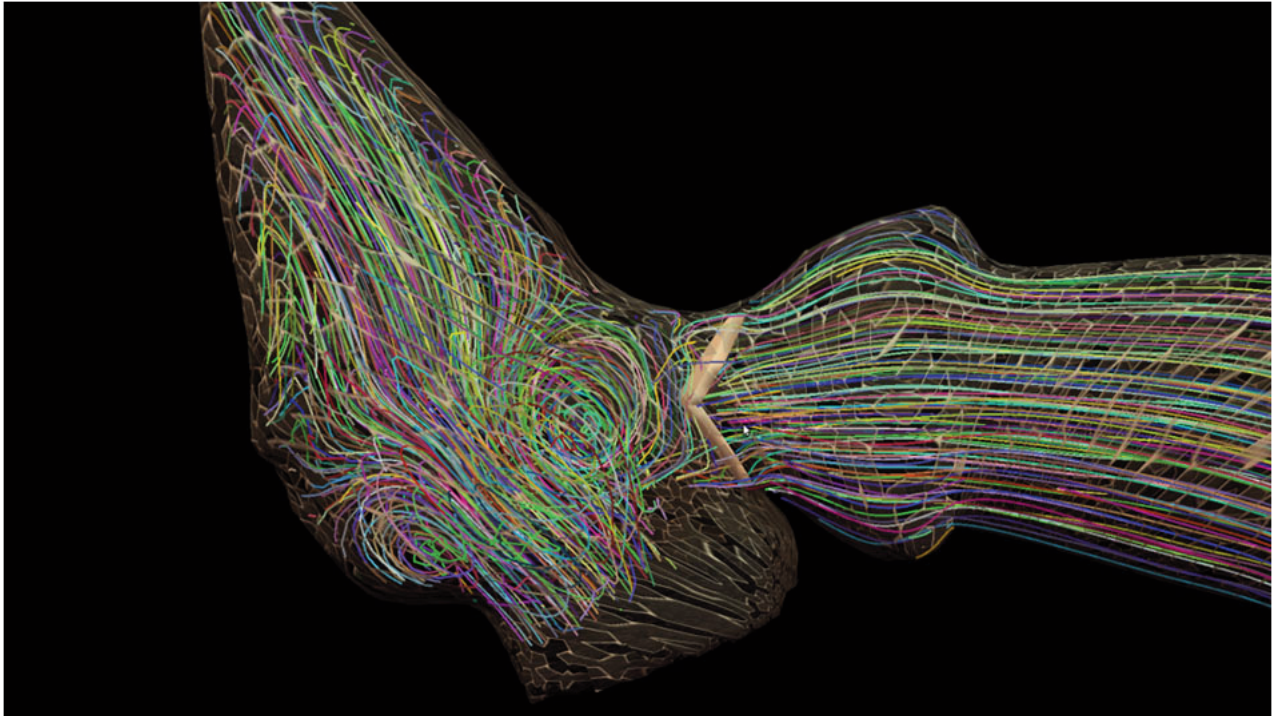
Also in This Issue

Figure 2. Groundbreaking fluid-solid interaction (FSI) models now make simulating accurate time-varying blood flow in patient specific geometries possible. The simulation describes flow through a synthetic heart valve as it opens and closes with the beat of the heart inside of a patient-specific model of the left ventricle and aorta.

tions, visualizing and comparing massive numbers of results, and interacting directly with the parameter space to explore new device designs. A schematic of this immersive simulation-based virtual design environment can be seen in Figure 1. In this vision, all of the components are backed by databases composed of pre-existing device models, patient-specific anatomies, and tissue properties. This design environment would enable a fundamentally new data-intensive workflow for device engineers to create initial designs and interactively refine them with the informed context provided by accurate simulation results. In partnership with the Minnesota Supercomputing Institute, three groups across campus have started to explore the research challenges associated with this new biomedical workflow and immersive envi-

ronment vision: the Interactive Visualization Lab in the Department of Computer Science and Engineering, the St. Anthony Falls Laboratory (SAFL), and the Medical Devices Center. Members of the team include: Dane Coffey (Computer Science), Trung Le (SAFL), Vamsi Konchada (Computer Science), Nicholas Malbraaten (Computer Science), Chi-Lun Lin (Mechanical Engineering), Yi Sun (Mechanical Engineering), Molly Staker (Mechanical Engineering), Iman Borazjani (SAFL), Victoria Interante (Computer Science), Daniel Keefe (Computer Science), Fotis Sotiropoulos (Director, SAFL), and Arthur Erdman (Mechanical Engineering; Director, Medical Devices Center). MSI staff who have contributed to this research include Nancy Rowe and H. Birali Runesha.

A high-performance simulation

framework has been developed to couple computational fluid dynamics (CFD) simulations with advanced fluid-solid interaction (FSI) models in order to simulate a heartbeat and the resulting opening and closing of mechanical valves implanted in the heart. Results from this work have established a new standard in physiologically accurate cardiovascular simulation. Figure 2 shows a visualization of simulated blood flow through a patient-specific model of the left ventricle and aorta extracted from CT imaging data. The researchers envision that the new power provided by simulations such as these can form the backbone of the interactive design environment outlined in Figure 1. In this vision of the future, where fast, accurate simulation is coupled with engineering design tools, the results of multiple simulations could be

compared using visualization to understand the impact of different design parameters on valve function and the three-dimensional geometry of the valve could be edited interactively by engineers.

To employ this style of simulation-based design workflow, new techniques for visualizing large, complex datasets are needed. Rapid increases in complexity and resolution of CFD simulation data parallel the exponential advances in supercomputing resources. However, a major bottleneck exists in conveying the information that results from these visualizations to users. Traditional desktop-based data visualizations struggle to convey the complex spatial relationships and other complexities in the data. In contrast, emerging

techniques for visualizing data using immersive virtual reality (VR) provide new opportunities for insights and discoveries that may have otherwise been missed. Using visualization environments, such as the MSI PowerWall shown in Figure 3 (located in the LCSE/MSI Visualization Laboratory), scientists and engineers can view simulation results from the perspective of a blood cell, investigating small-scale data features in detail. Interactive VR environments, such as this one, combine stereoscopic vision with three-dimensional head tracking to produce three-dimensional views of the data that update, recalculating the correct perspective projection of the three-dimensional scene, as scientists walk through the virtual

environment. In addition to room-sized VR environments, the team is also investigating the potential of smaller scale, more affordable VR environments constructed using commercially available three-dimensional televisions, which may provide the engineering workbench of the future.

In addition to the challenge of visualizing complex datasets, the new data-intensive workflow envisioned by the team also raises significant challenges for human-computer interaction, as the success of these visualizations depends heavily on the ability of engineers to explore their data, testing hypotheses and forming new hypotheses as they work. To better support visualization at the workbench scale, the team is new data

Figure 3. Immersive virtual reality (VR) visualizations provide scientists and engineers with new detailed views of complex anatomical geometries and data. Using the MSI PowerWall, results of a blood flow simulation through an aorta and synthetic heart valve can be explored interactively.
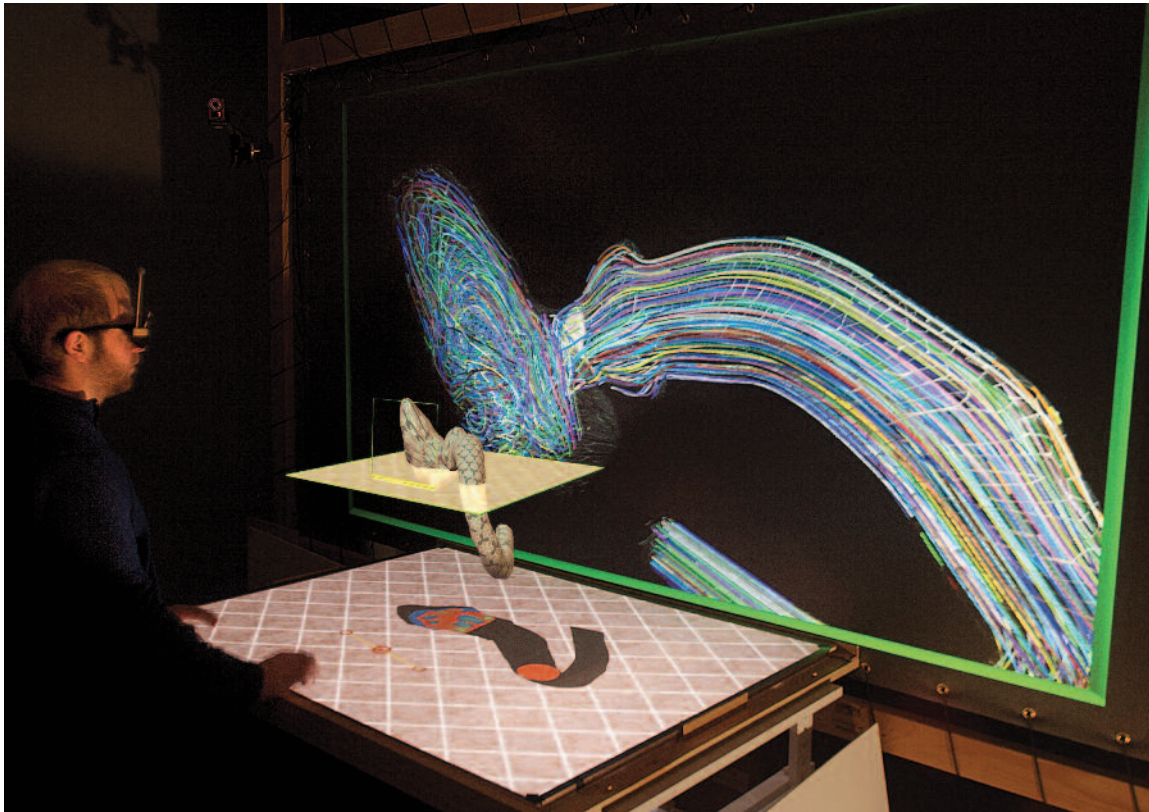
Figure 4. New human-computer interfaces are needed to support data exploration. Here a multi-touch table display is coupled with a VR display to provide new possibilities for interacting with data, such as manipulating three-dimensional data that appears (through stereoscopic projection) to float above the table by manipulating its shadow.

exploration interfaces that leverage emerging technologies, such as multi-touch input. Figure 4 shows a semi-immersive VR environment that is coupled with a large multi-touch table display. This environment makes it possible to explore complex three-dimensional datasets in using a variety of new interaction metaphors. For example, in the figure, the user navigates through complex three-dimension-al data from a blood flow simulation using rich multi-touch gestures made on top of an interactive shadow of the data displayed on the table. In addition to supporting rich input, the table display surface also provides a large visual surface capable of organizing and displaying additional information. In the future, the researchers expect that interactive visual data exploration environments such as this one will serve as the a medical device designer's workbench, enabling new modes of refining design iterations, spinning off high-resolution simulations, and organizing massive amounts of data, and, ultimately, leading to improved innovation and design of safe and effective medical devices.

2010 Undergraduate Internship Program

The Supercomputing Institute's Undergraduate Internship Program, now in its 20th 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. The program encompasses digital simulation and advanced computation and all aspects of high-performance computing and scientific modeling and simulation, as well as graphics, visualization, informatics, and high-performance network communications. Interns work with Principal Investigators at the Supercomputing Institute and their research groups on their projects. They give a presentation about their research to the intern group as well as the faculty and other researchers and also prepare a written report.

The Summer 2010 program included 11 interns who worked on projects in a wide variety of fields. They were selected from over 100 applicants at colleges and universities in the United States and Puerto Rico. Eight of the interns worked on projects sponsored by the Supercomputing Institute's Research Experiences for Undergraduates (REU) grant from the National Science Foundation (NSF), two were sponsored by internal MSI funds, and one was sponsored by his faculty mentor's NSF grant.

Bjorn K. Berntson, a University of Minnesota physics and mathematics double major, worked with Professor Christopher J. Cramer, Department of Chemistry and MSI Fellow. Mr. Berntson's project was titled "Electronic Structure Characterization of the $(bpy)_2MO_2$ Catalyst."

University of Minnesota chemistry major **Erik M. Fritz** worked with Professor Steven A. Kass, Department of Chemistry and Supercomputing Institute Fellow. Mr. Fritz, who was also in the 2009 intern program in the Kass group, worked on a project called "Energy Barriers and Relative Basicity."

Timothy M. Hecht was in the research group of Professor J. Woods Halley, Department of Physics and Supercomputing Institute Fellow. Mr. Hecht is a physics major with mathematics and business minors at Brigham Young University in Provo, Utah. His project was entitled "Electronic Spin Structures of Pt, O, and H With Possible Catalysis Applications."

Michelle S. Lenz, from Bethel University in St. Paul, Minnesota, worked with the research group of Regents Professor Donald G. Truhlar, Department of Chemistry

Michelle Lenz, Tim Hecht, Erik Fritz, and Bjorn Berntson at the intern program Welcome Luncheon.

Andrew Wesson gives his presentation.

Adam M. Novak, who attends Harvey Mudd College in Claremont, California, worked with Professor Victor Barocas, Department of Biomedical Engineering and Supercomputing Institute Fellow. Mr. Novak is a double major in computer science and biology, and his project was "Multi-scale Modeling on the GPU."

University of Minnesota mathematics major **David A. Sanchez** worked with Professor David A. Yuen, Department of Geology and Geophysics and Supercomputing Institute Fellow. His project was "2D and 3D Mantle Convection on the GPU."

Ashwin P. Srikrishna, who attends North Carolina State University in Raleigh, North Carolina, worked with Assistant Professor Kevin Dorfman, Department of Chemical Engineering and Materials Science and Supercomputing Institute Associate Fellow. Mr. Srikrishna majors in chemical engineering with a minor in nuclear engineering. Mr. Srikrishna's project was entitled "Parallelization of a Brownian Dynamics Simulation

and Supercomputing Institute Fellow. Ms. Lenz is an engineering science major with an emphasis in biomedical engineering, and her project was "Electrochemical Properties of Ruthenium Catalysts in Solution."

University of Minnesota neuroscience major **Aatif Mansoor** worked with Assistant Professor Elizabeth A. Amin, Department of Medicinal Chemistry and Super-

computing Institute Associate Fellow. His project was "Anthrax Toxin Lethal Factor Inhibitors: In Silico Design Approaches."

Brendan A. Murphy, a University of Minnesota biomedical engineering major, worked with Assistant Professor Tay I. Netoff, Department of Biomedical Engineering. His project was "Deep Brain Stimulation and Neuronal Synchrony."

Left to right: Andrew Wesson, Bjorn Berntson, Erik Fritz, Aatif Mansoor, Adam Novak, Michelle Lenz, Alexandra Zudova, Tim Hecht, Aaron Erdman, and Ashwin Shrikrishna.

of DNA Electrophoresis in a Non-homogeneous Electric Field."

Andrew J. Wesson attends Carnegie Mellon University in Pittsburgh, Pennsylvania, where he is a physics major. He worked in the research group of Professor Thomas W. Jones, Department of Astronomy, Supercomputing Institute Fellow, and Interim Director of the Institute until August 1, 2010. His project was "Radiative Cooling in Astrophysical Magneto-Hydrodynamic Simulations."

Alexandra M. Zudova, a University of Minnesota chemical engineering major with a chemistry minor, worked with Professor David D. Thomas, Department of Biochemistry, Molecular Biology, and Biophysics and MSI Fellow. Her project was "Molecular Dynamics Simulation of a Spin-labeled Membrane Protein."

While not a member of the formal program, **Aaron Erdman**, a student at Century College in White Bear Lake, Minnesota, participated in many of the intern program's activities during the summer. Mr. Erdman is a student in the Telecommunication Technology program at Century. He worked with MSI Scientific Computing Consultant Nancy Rowe on several projects at the LCSE-MSI Visualization Laboratory during the summer.

See the sidebar on this page for the announcement about next year's intern program.

Summer 2011
Undergraduate Internship Program

The Supercomputing Institute is pleased to announce its Undergraduate Internship Program for Summer 2011. Appointments are for full-time, 10-week internships, and will run from June 6 through August 12, 2011. A student interested in becoming an intern must still be an undergraduate in August 2011 and must be a citizen or permanent resident of the United States or its possessions. Interns will be paid a stipend of $5,000. Room and board at the University residence hall are free to the interns. If interns wish to live elsewhere, they will receive a per-diem food allowance and can request reimbursement for housing costs.

All applications are evaluated competitively based on the qualifications of the applicant and the availability of a suitable project. Projects are available in the following disciplines:

Aerospace Engineering and Mechanics
Astronomy
Biochemistry
Biomedical Engineering
Chemistry
Computer Science
Geology and Geophysics
Medicinal Chemistry
Physics

Complete application information, application forms, and project lists are available on the Supercomputing Institute website at:
www.msi.umn.edu/programs/undergraduateinternship.html

Applications, transcripts, and letters of recommendation can be emailed, faxed, or mailed as shown below.

Email: uip@msi.umn.edu
Fax: 612-624-8861
Mail: Undergraduate Internship Coordinator
                University of Minnesota
                Supercomputing Institute
                599 Walter
                117 Pleasant Street SE
                Minneapolis, MN 55455
Phone: (612) 624-2330

All applications and letters of recommendation must be received by February 28, 2011.

International Workshop on GPU Computing

David A. Yuen (Geology and Geophysics and MSI Fellow) was on the organizing committee for the 2010 International Workshop of GPU Solutions to Multiscale Problems in Science and Engineering, which was held in Harbin, China during Summer 2010. The two-day workshop included over 100 attendees from colleges, universities, and research centers from around the world. The attendees discussed such topics as GPU solutions to multi-scale problems, focusing on high-performance computing methods and algorithms, efficient software implementation technique, the construction of the scientific computing environment, and mainstream development

trends. Besides Professor Yuen, attendees from the University of Minnesota included MSI Scientific Computing Consultant Dr. Shuxia Zhang (shown above, giving a presentation), MSI Summer 2010 Undergraduate Intern David A. Sanchez (see article, page 5), and MSI Summer 2009 Undergraduate Intern Robin Weiss.

MSI Research Exhibition 2011

MSI will host a Research Exhibition poster session on April 29, 2011. All MSI researchers will be invited to present posters of their work using MSI resources. Prizes will be awarded to the outstanding posters.

The Call for Posters will be sent out in early February. We will post more information as it becomes available on the Research Exhibition 2011 website (*www.msi.umn.edu/events/researchexhibition2011.html*).

New Supercomputer, "Koronis"

MSI was recently awarded an NIH grant that is allowing us to purchase a new supercomputing system, which has been named "Koronis" after a lake in central Minnesota. Koronis features an SGI Altix UV 1000 supercomputer that has a shared-memory architecture in which each core can access all 3.1 terabytes of memory directly. Koronis also includes high-performance visualization workstations and high-performance and -fidelity data storage. This system will be used by MSI researchers working on a number of NIH-funded projects in the areas of multi-scale modeling, chemical dynamics, bioinformatics and computational biology, and biomedical imaging. The Principal Investigator on the grant is Professor Darrin York (Chemistry, MSI Fellow). Other major users of Koronis will include Jiali Gao (Chemistry, MSI Fellow), Donald Truhlar (Chemistry, MSI Fellow), George Karypis (Computer Science and Engineering, MSI Associate Fellow), David Largaespada (Genetics, Cell Biology, and Development), Kelvin Lim (Psychiatry), and Bin He (Biomedical Engineering). Koronis will also be available to other MSI researchers who have NIH funding.

Koronis was delivered in early October and is undergoing acceptance testing. It should be available for full-scale use in January 2011. Up-to-date information can be found on the MSI web-site as it becomes available: *www.msi.umn.edu/hardware/*

Welcome Reception for MSI Director

On September 14, MSI held a reception to formally welcome Jorge Viñals as the new Director of the Supercomputing Institute. Attendees included MSI researchers and staff, members of the staff of the Office of the Vice President for Research, supercomputing vendors, and other members of the MSI extended community. In the picture at right, Vice President for Research Tim Mulcahey makes a few welcoming remarks. Left to right: Jorge Viñals, H. Birali Runesha (MSI Assistant Director of Scientific Computing), Tim Mulcahey, Mike Balak (IT Director, CFANS), and Brian Ropers-Huilman (MSI Assistant Director of HPC Operations). At far right, back to camera, Mark Nelson (MSI HPC Systems Administrator).

Outreach Activities

MSI at the Minnesota State Fair

On September 2, 2010, MSI was at the Minnesota State Fair with the Medical Devices Center. Visitors to the University of Minnesota's building that day got to "fly through" a three-dimensional visualization of a heart. In the picture at right, MSI Visualization Specialist Mike Knox (right, in yellow shirt) talks to a fair visitor about what she's seeing onscreen. The visitor is wearing 3D glasses to view the image.

Math and Science Family Fun Fair

MSI participated in the College of Science and Engineering's Math and Science Family Fun Fair on Saturday, November 13. MSI staff members Yectli Huerta and Samantha Thomas and MSI PI Carlos Sosa and his son Daniel showed the visiting kids and their parents how supercomputers help researchers. The children were able to build model molecules and see how scientists use computers to make animated molecule simulations.

Visitors to the LCSE-MSI Visualization Laboratory

On October 14, two groups of middle-school students from the Washington Technology Magnet school in St. Paul, Minnesota visited the lab. These students are part of the BioSMART (Biologically focused Science, Math, Academic Rigor, and Technology) Program. The students watched three-dimensional visualizations on the LMVL's large screen and learned how doctors and scientists use these visualizations.

On October 21, students participating in "Body Forward," the 2010 Minnesota FIRST LEGO League robotics competition, visited the LMVL as part of the University of Minnesota Research Workshop. At left, Assistant Professor Matt Johnson (Biomedical Engineering, MSI Principal Investigator) shows the students how doctors can look at CAT scans in three dimensions. The students also got to participate in some hands-on virtual reality brain surgery. The University of Minnesota Research Workshop is hosted by the College of Science and Engineering. More information about FIRST LEGO League can be found at *www.firstlegoleague.org*.

On November 12, Dave Plescia, a representative from Johnson & Johnson, visited the University of Minnesota to discuss collaboration possibilities with University researchers involved in medical-device development. Professors Dan Keefe (Computer Science and Engineering), Fotis Sotiropoulos (Director, SAFL), and Art Erdman (Mechanical Engineering; Director, Medical Devices Center) and some of their students attended the presentation about Johnson & Johnson's medical devices. Mr. Plescia (pictured at right) also watched some of the visualizations currently being created using MSI resources.

Research Reports

Aerospace Engineering and Mechanics

2010/137
Dynamic k-Equation Model for Large Eddy Simulation of Compressible Flows
X. Chai and **K. Mahesh**

2010/138
Euler-Lagrangian Simulation of Bubble Migration in a Turbulent Boundary Layer
M. Mattson and **K. Mahesh**

2010/139
Simulations of High Speed Turbulent Jets in Crossflow
X. Chai and **K. Mahesh**

2010/140
Transition of Hypersonic Flow Past Flat Plate With Roughness Elements
P.S. Iyer, S. Muppidi, and **K. Mahesh**

2010/191
DNS of Transition in Supersonic Boundary Layers
S. Muppidi and **K. Mahesh**

Agronomy and Plant Genetics

2010/131 and CB 2010-44
An Integrative Approach to Genomic Introgression Mapping
A.J. Severin, G.A. Peiffer, W.W. Xu, D.L. Hyten, B. Bucciarelli, J.A. O'Rourke, Y.-T. Bolon, D. Grant, A.D. Farmer, G.D. May, **C.P. Vance**, R.C. Shoemaker, and **R.M. Stupar**

2010/146 and CB 2010-49
Transcriptome Analysis of the Barley–Deoxynivalenol Interaction: Evidence for a Role of Glutathione in Deoxynivalenol Detoxification
S.A. Gardiner, J. Boddu, F. Berthiller, C. Hametner, **R.M. Stupar**, G. Adam, and G.J. Muehlbauer

2010/147 and CB 2010-50
The Genetics of Barley Low-Tillering Mutants: Low number of Tillers-1 (lnt1)
T. Dabbert, R.J. Okagaki, S. Cho, S. Heinen, J. Boddu, and **G.J. Muehlbauer**

2010/148 and CB 2010-51
Structural and Functional Characterization of a Winter Malting Barley
M. Munoz-Amatriain, L. Cistue, Y. Xiong, H. Bilgic, A.D. Budde, M.R. Schmitt, **K.P. Smith**, P.M. Hayes, and **G.J. Muehlbauer**

2010/172 and CB 2010-63
*Transcript Profiling of Common Bean (*Phaseolus vulgaris L.*) Using the GeneChip Soybean Genome Array: Optimizing Analysis by Masking Biased Probes*
S.S. Yang, O. Valdes-Lopez, W.W. Xu, B. Bucciarelli, **J.W. Gronwald**, G. Hernandez, and **C.P. Vance**

2010/173 and CB 2010-64
Transcript Profiling of Two Alfalfa Genotypes With Contrasting Cell Wall Composition in Stems Using a Cross-Species Platform: Optimizing Analysis by Masking Biased Probes
S.S. Yang, W.W. Xu, M. Tesfaye, J.F.S. Lamb, H.J.G. Jung, K.A. VandenBosch, **C.P. Vance**, and **J.W. Gronwald**

Animal Science

2010/134 and CB 2010-45
Genome-Wide Association Analysis of Total Cholesterol and High-Density Lipoprotein Cholesterol Levels Using the Framingham Heart Study Data
L. Ma, J. Yang, H. B. Runesha, T. Tanaka, L. Ferrucci, S. Bandinelli, and **Y. Da**

Biochemistry, Molecular Biology, and Biophysics

2010/89 and CB 2010-34
Structural Insight Into Methyl-Coenzyme M Reductase Chemistry Using Coenzyme B Analogues
P.E. Cedervall, M. Dey, A.R. Pearson, S.W. Ragsdale, and **C.M. Wilmot**

2010/90 and CB 2010-35
Structural Features Promoting Dioxygen Production by Dechloromonas aromatica *Chlorite Dismutase*
B.R. Goblirsch, B.R. Streit, J.L. DuBois, and **C.M. Wilmot**

2010/91 and CB 2010-36
Kinetic and Structural Analysis of Substrate Specificity in Two Copper Amine Oxidases From Hansenula polymorpha
C.M. Chang, V.J. Klema, B.J. Johnson, M. Mure, J.P. Klinman, and **C.M. Wilmot**

2010/92 and CB 2010-37
In Crystallo *Posttranslational Modification Within a MauG/Pre-Methylamine Dehydrogenase Complex*
L.M.R. Jensen, R. Sanishvili, V.L. Davidson, and **C.M. Wilmot**

2010/149 and CB 2010-52
Phosphorylation-Induced Structural Changes in Smooth Muscle Myosin Regulatory Light Chain
D. Kast, L.M. Espinoza-Fonseca, C. Yi, and **D.D. Thomas**

Names of Supercomputing Institute principal investigators appear in bold type. This list contains reports entered into the reports database during August–November 2010.

Research Reports

2010/169 and CB 2010-60
Synthesis, Properties, and Applications of Diazotrifluropropanoyl-Containing Photoactive Analogs of Farnesyl Diphosphate Containing Modified Linkages for Enhanced Stability
M.L. Hovlid, R.L. Edelstein, O. Henry, J. Ochocki, A. DeGraw, S. Lenevich, T. Talbot, V.G. Young, A.W. Hruza, F. Lopez-Gallego, N.P. Labello, C.L. Strickland, **C. Schmidt-Dannert**, and **M.D. Distefano**

2010/200 and CB 2010-80
LTQ-iQuant: A Freely Available Software Pipeline for Automated and Accurate Protein Quantification of Isobaric Tagged Peptide Data From LTQ Instruments
G. Onsongo, M.D. Stone, S.K. Van Riper, J. Chilton, B. Wu, L. Higgins, T.C. Lund, **J.V. Carlis**, and **T.J. Griffin**

BioTechnology Institute

2010/145 and CB 2010-48
Switching From an Esterase to a Hydroxynitrile Lyase Mechanism Requires Only Two Amino Acid Substitutions
S.K. Padhi, R. Fujii, G.A. Legatt, S.L. Fossum, R. Berchtold, and **R.J. Kazlauskas**

Center for Drug Design

2010/93 and CB 2010-38
Dual Inhibitors of Inosine Monophosphate Dehydrogenase and Histone Deacetylase Based on a Cinnamic Hydroxamic Acid Core Structure
L. Chen, R. Petrelli, G. Gao, D.J. Wilson, G.T. McLean, H.N. Jayaram, **Y.Y. Sham**, and K.W. Pankiewicz

2010/168 and CB 2010-59
N-3 Hydroxylation of Pyrimidine-2,4-diones Yields Dual Inhibitors of HIV Reverse Transcriptase and Integrase
J. Tang, K. Maddali, C.D. Dreis, **Y.Y. Sham**, R. Vince, Y. Pommier, and Z. Wang

Chemical Engineering and Materials Science

2010/104
Koopmans' Condition for Density-functional Theory
I. Dabo, A. Ferretti, N. Poilvert, Y. Li, N. Marzari, and **M. Cococcioni**

2010/113
Dynamics of Surface Structure Evolution in Colloidal Adsorption: Charge Patterning and Polydispersity
D.D. Brewer, **M. Tsapatsis**, and **S. Kumar**

2010/133
Accurate and Efficient Calculations on Strongly Correlated Minerals With the LDA+U Method: Review and Perspectives
M. Cococcioni

2010/136
Tuning the Charge-Transport Parameters of Perylene Diimide Single Crystals via End and/or Core Functionalization: A Density Functional Theory Investigation
M.C. Ruiz Delgado, E.-G. Kim, D.A. da Silva Filho, and J.-L. Bredas

2010/174
Existence, Stability, and Nonlinear Dynamics of Detached Bridgman Growth States Under Zero Gravity
A. Yeckel and **J.J. Derby**

2010/176 and CB 2010-67
Free Energy Profile of the Interaction Between a Monomer or a Dimer of Protegrin-1 in a Specific Binding Orientation and a Model Lipid Bilayer
V. Vivcharuk and **Y. Kaznessis**

2010/177 and CB 2010-66
Antimicrobial Mechanism of Pore-forming Protegrin Peptides: 100 Pores to Kill E. coli
D. Bolintineanu, E. Hazrati, H.T. Davis, R.I. Lehrer, and **Y.N. Kaznessis**

2010/192
Quasiharmonic Thermal Elasticity of Crystals: An Efficient Analytical Approach
Z. Wu and **R.M. Wentzcovitch**

2010/193
The Hubbard U Correction for Iron-Bearing Minerals: A Discussion Based on $(Mg,Fe)SiO_3$ Perovskite
H. Hsu, K. Umemoto, **M. Cococcioni**, and **R.M. Wentzcovitch**

2010/194
Thermodynamic Properties of $MgSiO_3$ Majorite and Phase Transitions Near 660-km Depth in $MgSiO_3$ and Mg_2SiO_4: A First Principles Study
Y.G. Yu, **R.M. Wentzcovitch**, V.L. Vinograd, and R.J. Angel

2010/195
Effect of the d Electrons on Phase Transitions in Transition-Metal Sesquioxides
K. Umemoto and **R.M. Wentzcovitch**

Chemical Engineering, UMD

2010/197
Combined Gravitational and Thermocapillary Interactions of Spherical Drops With Incompressible Surfactant
M.A. Rother

Chemistry

2010/95 and CB 2010-41
Equilibrium Mercury Isotope Fractionation Between Dissolved Hg(II) Species and Thiol-Bound Hg
J.G. Wiederhold, **C.J. Cramer**, K. Daniel, I. Infante, B. Bourdon, and R. Kretzschmar

2010/96 and CB 2010-40
High Tg Aliphatic Polyesters by the Polymerization of Spirolactide Derivatives
G.L. Fiore, F. Jing, V.G. Young, Jr., **C.J. Cramer**, and **M.A. Hillmyer**

Research Reports

2010/97
Prediction of SAMPL2 Aqueous Solvation Free Energies and Tautomeric Ratios Using the SM8, SM8AD, and SMD Solvation Models
R.F. Ribeiro, A.V. Marenich, **C.J. Cramer**, and **D.G. Truhlar**

2010/126
Enolates in 3-D: An Experimental and Computational Study of Deprotonated 2-Adamantanone
M.M. Meyer and **S.R. Kass**

2010/127 and CB 2010-43
An Infrared Multiphoton Dissociation Spectroscopy Study of Protonated p-Aminobenzoic Acid: Does Electrospray Ionization Afford the Amino- or Carboxy-Protonated Ion?
J. Schmidt, I. Spector, M.M. Meyer, and **S.R. Kass**

2010/135 and CB 2010-46
Internal Proton Transfer in the External Pyridoxal 5'-Phosphate Schiff Base in Dopa Decarboxylase
Y. Lin and **J. Gao**

2010/152 and CB 2010-54
Tunneling in Enzymatic and Nonenzymatic Hydrogen Transfer Reactions
D.G. Truhlar

2010/153
Tests of the RPBE, revPBE, τ-HCTHhyb, ωB97X-D, and MOHLYP Density Functional Approximations and 29 Others Against Representative Databases for Diverse Bond Energies and Barrier Heights in Catalysis
K. Yang, J. Zheng, Y. Zhao, and **D.G. Truhlar**

2010/154
Density Functional Study of CO and NO Adsorption on Ni-doped MgO(100)
R. Valero, J.R.B. Gomes, **D.G. Truhlar**, and F. Illas

2010/155 and CB 2010-53
Kinetics of Hydrogen-Transfer Isomerizations of Butoxyl Radicals
J. Zheng and **D.G. Truhlar**

2010/156
Binding Energy of d^{10} Transition Metals to Alkenes by Wave Function Theory and Density Functional Theory
B.B. Averkiev, Y. Zhao, and **D.G. Truhlar**

2010/157 and CB 2010-55
Density Functional Calculations of E2 and S_N2 Reactions: Effects of the Choice of Density Functional, Basis Set, and Self-Consistent Iterations
Y. Zhao and **D.G. Truhlar**

2010/158
On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies
D. Jacquemin, E.A. Perpete, I. Ciofini, C. Adamo, R. Valero, Y. Zhao, and **D.G. Truhlar**

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