

Broader Engagement Session Schedule & Abstracts



SUNDAY, NOVEMBER 16, 2008

10:30 AM – 11:15 AM

Joe Marks, VP-R&D, Walt Disney Imagineering & Walt Disney Animation Studios

The Challenges and Opportunities of Entertainment Computing

Digital storytelling is a major part of our culture and our economy. Computing technology is changing how stories are authored and how they are experienced. I will describe several areas in which telling the story poses some unusual computational challenges:

- Physical simulation for cloth, hair, and fluids.
- Computational cinematography.
- New display technologies.
- Mobile applications in parks, arenas, and cinemas.
- Sports visualization.

Joe Marks grew up on the Northside of Dublin before emigrating to the U.S. to attend college. He holds three degrees from Harvard University. His areas of interest include computer graphics, human-computer interaction, and artificial intelligence. He has worked previously at Bolt Beranek and Newman, Digital's Cambridge Research Laboratory, and Mitsubishi Electric Research Labs (MERL), where he was Research Director from 2000-2006. He is currently Vice President for R&D at Walt Disney Imagineering and Walt Disney Animation Studios.

11:15 AM – 12:00 PM

M. Brian Blake, Department of Computer Science, Georgetown University

Being Faculty: A View from the Trenches

Nine years serving as a faculty member in a computer science department is perhaps not a long time in an academic sense. However, it does represent a good milestone by which to reflect on the challenges of navigating the tenure-track and the aspiration to be successful in the full professor promotion track. In a significantly practical way, this talk attempts to illuminate the benefits of being a faculty member and challenges that lie ahead. In targeting graduate students and early faculty members, this talk can be summarized as 3 reasons to become a professor and 4 mistakes that I hope you avoid. In addition, these experiences are flavored with the integration of diversity.

M. Brian Blake is an Associate Professor and Chair in the Department of Computer Science at Georgetown University. Dr. Blake conducts applied research in the development of automated approaches for the sharing of information and capabilities across organizational boundaries, sometimes referred to as enterprise integration. With respect to this area of interest, his investigations cover the spectrum of software systems engineering: design, specification, proof of correctness, implementation/experimentation, performance evaluation, and application. He has published over 85 journal articles and refereed conference papers in the areas of service-oriented computing, intelligent agents and workflow, enterprise systems integration, component-based software engineering, distributed data management, and software engineering education. Over the past 7 years, his research lab has been awarded over \$5.5 million in sponsored research from the National Science Foundation, DARPA, Federal Aviation Administration, the MITRE Corporation, Air Force Research Lab, SAIC, and the National Institute of Health. Dr. Blake received a Bachelor of Electrical Engineering from Georgia Institute of Technology and PhD in Information and Software Engineering from George Mason University. More information about Dr. Blake can be found at <http://www.cs.georgetown.edu/~blakeb/>

1:30 PM – 2:15 PM

PANEL: Dona Crawford, Barbara Horner-Miller, Janet Jacobsen, Becky Verastegui

Meeting the Challenges that Face the Nation – National Labs and Supercomputing Centers

High Performance Computing plays a pivotal role in science and research today. Scientific discoveries made possible through large-scale simulations address many of the challenges we face - understanding the climate changes that lead to global warming, creating renewable and sustainable energy sources, addressing national and global security concerns, and improving health through the study of disease vectors and genetic factors - as well as enable us to advance our understanding of fundamental science such as studying the life and death of stars and the structure of the universe. This panel will highlight the computational research at various National Laboratories and Supercomputing Centers and how these research hubs are meeting the challenges that face the nation.

Dona Crawford, Associate Director, Computation Directorate, LLNL

Dona has 31 years of computational management experience at Lawrence Livermore (LLNL) and Sandia National Laboratories. As Associate Director for Computation at LLNL starting in 2001, she has responsibility for a staff of roughly 1000 who develop and deploy an integrated computing environment for terascale simulations of complex physical phenomena. This environment includes high-performance computers, scientific visualization facilities, high-performance storage systems, network connectivity, multiresolution data analysis, mathematical models, scalable numerical algorithms, computer applications and services that enabled LLNL mission goals and scientific discovery. Icons for the computing environment provided include the Advanced Simulation and Computing (ASC) Program's BlueGene/L machine and the ASC Purple machine. Both are among the fastest computers in the world. Ms. Crawford has served on advisory committees for the National Research Council, the National Science Foundation, and the Council on Competitiveness. She is active in the SC conference series and participates in community outreach activities to promote math and science. Crawford received the Computerworld Honors Award (2006) and was named 2005 Woman of the Year in Science in Alameda County. She received a master's degree in operations research from Stanford University and a bachelor's degree in mathematics from the University of Redlands, Calif.

Barbara Horner-Miller, Associate Director, ARSC

Barbara has 40 years of experience in the computing field. Her leadership and knowledge of the High Performance Computing community is demonstrated by her career advancement and her professional activities in the SC and CUG communities. The first part of her career was spent working with scientists and engineers programming to solve computational problems using state-of-the-art computers at world-class institutions: The Rand Corporation, the National Center for Atmospheric Research, NASA's Jet Propulsion Laboratory and the Arctic Region Supercomputing Center. From 1978-2005, she worked in User Services organizations of these institutes in positions of increasing scope and responsibility. Since 2005, she has been Director of Computational Services at the Arctic Region Supercomputing Center. In this position she directs the support staff of the center. During her career, she has frequently served as a liaison between her organization and other industry, government and educational organizations. She served as Chair of SC2006.

Janet Jacobsen, Visualization and Analytics Engineer, LBNL/NERSC

Janet has been developing software to support research efforts in a variety of scientific disciplines for nearly 25 years. Currently, she is a member of the LBNL High-Performance Computational Research Division's Visualization Group and deputy team lead for the NERSC Analytics Group. Jacobsen received her M.A. in mathematics and B.A. in applied mathematics and statistics from UC Berkeley. While in graduate school, she joined the Earth Sciences Division at LBNL as a computing technician, and later became a staff scientist. While working in the earth sciences, she analyzed field data, developed finite element mesh generators for fracture data and numerical simulators for reactive chemical transport, and developed visualizations involving many types of field data in support of the Department of Energy's (DOE) high-level nuclear waste isolation program and other geosciences program. Jacobsen developed pre- and post- processing visualizations for CFD code while working as a computer scientist/mathematician in the Atmospheric Research Division at LLNL. Thereafter, she moved to UC Berkeley

where she she was a programmer/analyst for the Engineering Systems Research Center and the Institute for Quantitative Biomedical Research. While at UC Berkeley, Jacobsen developed software tools to manage, display, and analyze data and metadata for low- and high-throughput microbiology experiments in support of DOE's Genomics:GTL Program. She currently works with other members of the NERSC Analytics Group to help NERSC users analyze and visualize simulation and experimental data.

Becky Verastegui, Director, Information Technology Services Division, ORNL

Becky is Director of the Information Technology Services Division at Oak Ridge National Laboratory. The Division provides strategic information technology solutions for ORNL's diverse business and scientific information infrastructure. Her Division provides data and voice networks, email and web infrastructure, business systems, and all the support aspects of the Lab's IT infrastructure including cyber and information security, computer helpline, workstation and desktop support, applications programming, and computer operations. In 2007, Becky was the Chair of the SC07 Conference and currently serves as Chair Conference's Steering Committee. She is also Co-Chair of Exhibits for SC08. She has been keynote speaker and panelist at several national information technology conferences and has coauthored several magazine articles and strategic planning documents. Becky has worked at DOE's Oak Ridge facilities for over 30 years in a variety of computing-related positions. She has won several ORNL Awards Night awards and Lockheed Martin Corporation's NOVA award honoring her leadership and outstanding contributions toward realization of information technology advances. Becky has also received an award from Government Computing News for her leadership in DOE's long-range strategic planning and acquisition management processes, a DOE Headquarters Citation for Special Achievement in Information Resources Management Planning, and DOE-Oak Ridge Operations recognition for Significant Contributions.

2:15 PM – 3:00 PM

PANEL: Clint Dawson, Roscoe Giles, Raquell Holmes

What Would a Conversation of HPC Look Like if You Were in it?

"Exactly what is High Performance Computing (HPC) and who does it?" can be answered in many ways. In this session, the audience is introduced to HPC and HPC leaders through panel discussion and theatrical improvisational performance. The panel consisting of computer science researchers and HPC community builders will introduce their areas of interest, how their particular focus relates to HPC, and the role of community and diversity in their research lives and success in HPC. Student contributions will be used to direct improvisational conversations on HPC; improvisation provides a cultural opportunity to play with the socio-cultural aspects of HPC research and education. Brought to you by the Empowering Leadership: Computing Scholars of Tomorrow (EL) Alliance, <http://www.empoweringleadership.org>

Clint Dawson, University of Texas, Austin

Clint Dawson is a Professor of Aerospace Engineering and Engineering Mechanics, University of Texas, Austin. His research interests include development, analysis, and implementation of numerical methods for flow and transport in porous media and shallow water equations. Of particular interest are Discontinuous Galerkin schemes, finite volume schemes, and multialgorithmic strategies. Other interests include data assimilation and a posteriori error estimation. He is a member of the Leadership Team for the EL Alliance.

Roscoe Giles, Boston University

Roscoe Giles is the Deputy Director of the Center for Computational Science, Professor of Computer and Electrical Engineering, Boston University. His research focuses on applications of parallel supercomputers to physics and materials problems. He also works in computational science education. He is on the Leadership Team for the EL Alliance and co-director of the Boston University MARINER project. He was the general chair for the SC02 conference in Baltimore, Maryland, and in 2004, he was selected as one of the 50 Most Important Blacks in Research Science by the Science Spectrum Magazine and Career Communications Group, Inc.

Raquell Holmes, Boston University and University of Connecticut Health Center

Raquell Holmes is an Assistant Research Professor at Boston University. She is trained as a cell biologist, who has spent more than eight years managing computational science education and outreach programs to increase the use of HPC by biology researchers. She recently joined the Center for Cell Analysis and Modeling, home to the Virtual Cell, a publicly available Web-based application used to study cellular dynamics. Through workshops and publications, she introduces numerical modeling and modeling frameworks to experimentalists and students. She has simultaneously trained in using improvisation and performance to build collaborative learning environments with youth and adults.

3:30 PM – 4:15 PM

PANEL: Jose Castillo, Dilma da Silva, Michael Lee

Financing your Graduate Study: Graduate student opportunities & funding

Many students, especially women and students from underrepresented groups, don't realize that graduate school is a viable option. Funds for graduate study are available. The goal of this panel is to give students a glimpse into the graduate school experience and provide valuable information on the funding opportunities available to students in computing. The speakers (from universities, industry and a current graduate school student) will give a brief overview of some of the top funding sources available (i.e. institutions, fellowships and research and teaching support).

Jose Castillo, San Diego State University, Computational Science Research Center

Jose is director of the San Diego State University Computational Science Research Center and Professor in the Department of Mathematics and Statistics. This center facilitates cooperation between the University and Industry as well as National Laboratories. The center involves participation of researchers from applied mathematics, computer science, astronomy, physics, geophysics, and engineering. Dr. Castillo received his PhD in Applied Mathematics in 1987 from the University of New Mexico. He has a wide range of interests in applied mathematics with emphasis in numerical solution of partial differential equations, scientific computing, and modeling. His numerical interests are mainly in the solution of partial differential equations in irregular geometries with emphasis on grid generation for both geometry and solution adaption. He has developed new grid generation algorithms based on intuitive discrete geometric notions and has built codes to implement these ideas. He has studied the underlying mathematics including existence and uniqueness, and smoothness properties of the variational problems. He has an ongoing cooperation with the CNLS and the T7 group at Los Alamos National Laboratory with research projects involving High Order Finite Difference Schemes, Error analysis and Adaptive Grid Generation methods. DOE via Summer Fellowships has funded this research at Los Alamos National Laboratory.

Dilma da Silva, IBM T. J. Watson Research Center, NY

Dilma manages the Advanced Operating Systems group. She received her Ph.D in Computer Science from Georgia Tech in 1997. Prior to joining IBM, she was an Assistant Professor at University of Sao Paulo, Brazil. Her research in operating systems addresses the need for scalable and customizable system software. She has also worked in parallel computing, mobile computing, and software engineering. She has published more than 60 technical papers. More information can be found at www.research.ibm.com/people/d/dilma

Michael Lee, University of Kentucky

Michael is the Director of The Kentucky, West Virginia – Louis Stokes Alliance for Minority Participation (KYWV-LSAMP) at the University of Kentucky. The KYWV-LSAMP is a multidisciplinary undergraduate program featuring an organizational structure of multiple institutions working together toward a shared goal. The alliance includes partners from two- and four-year degree granting higher education institutions (10), business and industries, national research laboratories, and local, state, and federal agencies. The overarching aim of the partnership is to significantly increase the quantity and quality of underrepresented/underserved burgeoning population students who graduate from college with a degree in science, technology, engineering, or mathematics (STEM) disciplines. Lee serves on the Martin L. King Committee, and the President's Commission on Diversity (PCD) at the University of

Kentucky, and as a member of the Diversity Steering Committee at Georgetown College, Georgetown, KY. Lee is also an active member of many national organizations including the National Association of Multicultural Engineering Program Administrators. Lee has spent most of his professional career in higher education and led the way in creating diversity programs in New Mexico and Missouri including one project that the President of the United States (Ronald Reagan) Deemed "One of 19 exemplary programs meeting the needs of the Nation in STEM subject areas". This program model was exported to 16 states around the nation to include Majority Institutions, Historically Black Colleges and Universities (HBCU's), Hispanic Serving Institutions (HSI's), and Tribal Colleges (TC's). In addition to the KYWV-LSAMP Michael Lee is the proprietor of the New Mexico Community Faith Links a not-for-profit organization that customizes academic support constructs incorporating Social and Emotional Intelligence (SQ & EQ). He has recently published a co-curricular program-wide approach to learning called Social, Emotional, and Academic Learning (SEAL), with a great portion of his work exported to the Virgin Islands. In 2007, Michael Lee was awarded a Lifetime Achievement Award by the Governor of New Mexico Bill Richardson for his contribution to education.

4:15 PM – 5:00 PM

PANEL: Dorian Arnold, Jamika D. Burge, Christopher Harris, Lorie M. Liebrock

Graduate School – Front to Back

There is a large gap in knowledge and experience between undergraduate and graduate students. Expectations, available resources, and evaluation criteria for a graduate student differ greatly from the undergrad experience. This panel will address how one successfully makes the transition from undergraduate to graduate student, navigates the major challenges of life as a grad student, and gains the skills necessary to be successful in the post-grad school workforce. Panelists will bring insight on the grad student experience from the perspective of current PhD students, recent PhD recipients, and current and former PhD mentors.

Dorian Arnold, University of Wisconsin

Dorian is completing his Ph.D. this fall in the Computer Sciences Department at the University of Wisconsin where he was an Intel Graduate Fellow from 2006-2008. His current research interests are in large-scale distributed and Grid systems with a focus on the reliability and scalability of high-performance distributed tools and applications. In the spring of 2009 he will join the faculty of the Department of Computer Science at the University of New Mexico.

Jamika D. Burge, Pennsylvania State University

Jamika is currently a Postdoctoral Research Scholar in the College of Information Sciences and Technology at The Pennsylvania State University, University Park. She is managing a wireless network research project under the guidance of John M. Carroll at Penn State University. Burge completed her PhD in Computer Science from Virginia Polytechnic Institute and State University (Virginia Tech) in Blacksburg, VA. She has received several awards, including IBM PhD Research Fellow (2005-2006), and she has served in several leadership positions, including president of the Computer Science Graduate Student Council while at Virginia Tech. She continues to be a research mentor to undergraduate and graduate students. Burge is affiliated with several professional organizations, including the Association for Computing Machinery (ACM), and the CSE (Computer Science Education) and CHI (Computer-Human Interaction) Special Interest Groups.

Christopher Harris, University of California, Irvine

Christopher received B.S. degrees in Applied Mathematics and Computer Engineering in 1998 from Oakwood College and the University of Alabama in Huntsville, respectively. In 2001 he was awarded the M.S. degree in Electrical Engineering from the University of Notre Dame. After several years in industry, Harris returned to academia where he is currently pursuing a Ph.D. in Electrical Engineering and Computer Science at the University of California, Irvine under the advisement of Dr. Nader Bagherzadeh. Harris' current research interests include fault-tolerant computing, post-CMOS computer architectures, and reconfigurable computing. Harris is a member of the Tau Beta Pi and Eta Kappa Nu Engineering Honor Societies as well as the Alpha Chi National College Honor Society.

Lorie M. Liebrock, New Mexico Institute of Mining and Technology in Socorro, New Mexico

Lorie is an Associate Professor of Computer Science at New Mexico Institute of Mining and Technology. She is the Associate Chair for Undergraduate Affairs in the Department of Computer Science. She is also the Interim Education Director for the New Mexico Computing Applications Center for the State of New Mexico. She holds an M.S. and Ph.D. from Rice University and B.S. and M.S. from Michigan Technological University. Her research interests include foundations of computer science, information assurance, parallel processing, and visualization. She is particularly interested in complex problems that require the integration of all of these aspects of computer science.

MONDAY, NOVEMBER 17, 2008

9:00 AM – 10:00 AM

Valerie E. Taylor, Texas A&M

Universal Computational Science Education: Challenges and Opportunities

Today, with the availability of processors with multiple cores or multicore processors, all computer systems, even the home computers, include parallel processing. We are seeing an increase in the number of cores per processor with future computer chips. Further, many applications include significant computations for multi-media displays in addition to control decisions. Hence, it is important that our students are exposed to parallel processing or computational science education as early as possible. Such exposure should excite students about the field of computational science, with special focus on the engagement of underrepresented groups in math and science. Given the use of computers in so many disciplines, exposure to computational science is important for students to be leaders in their careers.

Valerie earned her B.S. in Electrical and Computer Engineering and M.S. in Computer Engineering from Purdue University in 1985 and 1986, respectively, and a Ph.D. in Electrical Engineering and Computer Science from the University of California, Berkeley, in 1991. From 1991 through 2002, Dr. Taylor was a member of the faculty in the Electrical and Computer Engineering Department at Northwestern University. Dr. Taylor joined the faculty of Texas A&M University as Head of the Dwight Look College of Engineering's Department of Computer Science in January of 2003, and is, also, currently a holder of the Royce E. Wisenbaker Professorship. Her research interests are in the areas of computer architecture and high performance computing, with particular emphasis on mesh partitioning for distributed systems and the performance of parallel and distributed applications. She has authored or co-authored over 100 papers in these areas. Dr. Taylor has received numerous awards for distinguished research and leadership, including the 2002 IEEE Harriet B. Rigas Award for a woman with significant contributions in engineering education, the 2002 Outstanding Young Engineering Alumni from the University of California at Berkeley, the 2002 CRA Nico Habermann Award for increasing the diversity in computing, and the 2005 Tapia Achievement Award for Scientific Scholarship, Civic Science, and Diversifying Computing. Dr. Taylor is a member of ACM and Senior Member of IEEE-CS.

10:30 AM – 11:15 AM

Thomas M. DeBoni

What's Wrong with Parallel Computing?

Parallel computing is difficult to do. Many characteristics of what we now call High Performance Capability Computing have arisen in the past 20 years, and most of them have contributed at least as much to the overall problem as to the solution: they've made computing faster and more difficult at the same time. Why is this? And is there anything we can do about it? This talk will briefly describe the extent of the problem, and then suggest potential solutions. There will be entertainment along with the pessimism.

Thomas has studied and worked in parallel computing since beginning his career at Livermore in 1979, when HPC meant vector processing. Since then, he has been involved in scientific computing, computer architectures, and programming languages, studied and taught at several major universities, and worked and published at three major laboratories. During this work, he has acquired definite opinions as to what the real problems are, why they exist, and what might be done about them.

11:15 AM – 12:00 PM

Dean Williams, LLNL

Climate Change: Current Knowledge and Future Challenges

3D stereo animation of 220 years of science observation and computer simulated global warming. The animation is derived directly from the Coupled Model Intercomparison Project 3 multi-model data archive that contributed to the Intergovernmental Panel on Climate Change (IPCC) fourth assessment report. Such efforts were recognized in the collective award of the 2007 Nobel Peace Prize to the IPCC scientific community (shared with former Vice President Albert Gore)—“for efforts to build up and disseminate greater knowledge about man-made climate change, and to lay the foundations for the measures that are needed to counteract such change”. This specific animation is a multi-model mean of 23 climate models, which projects surface temperature change, sea-ice at the poles, and cloud fractions spanning 220 years—from 1880 through 2100. The projection is based on a scenario in which little control is imposed on greenhouse gas emissions. This particular animation has not appeared anywhere before, but the data has been used to publish over 480 journal articles. To view the list of publications, please visit the following URL: http://www-pcmdi.llnl.gov/ipcc/subproject_publications.php.

Dean N. Williams is currently working at Lawrence Livermore National Laboratory (LLNL) as the lead computer scientist for the Program for Climate Model Diagnosis and Intercomparison (PCMDI). He has been with PCMDI for the past 19 years designing and developing data analysis tools and visualization. He has published and co-authored several technical papers in the area of visualization and data analysis tools and has had some of his work presented in books. He has been the lead developer of the Visualization and Computation System and is currently the lead developer of the Climate Data Analysis Tools. Dean was the initiator and important contributor of research proposals that received funding from the DOE Office of Science and the High Performance Computing and Communications (HPCC) Program. In addition, he has served as PI or co-PI on other research projects funded by LLNL's LDRD program. For the past seven years, Dean has been engaged in research in computer science focusing on high-performance and distributed computing, and climate analysis tools. The goal of Dean's work is to enhance interoperability between common climate analysis tools, and to enable end-to-end simulation and analysis workflow for the Earth Sciences communities.

1:30 PM – 2:15 PM

Olga Pearce, Texas A&M

Load imbalance in multi-physics simulations: Computer science to the rescue

Computer simulations allow us to mathematically model natural systems in physics, biology, and chemistry. Scientists model atoms in material deformation, molecular movement in protein folding, and molecular interaction in brain simulations to learn about systems that are hard to observe experimentally. Utilizing powerful supercomputers allows scientists to run simulations at an unprecedented level of detail and discover previously unknown phenomena, making performance of said applications crucial to furthering the discoveries. Unfortunately, it is common for simulations to suffer from a variety of performance problems such as uneven distribution of work between the processors, known as load imbalance. In this talk, we describe how load imbalance can be detected, analyzed, and corrected. We use a large multi-physics simulation at LLNL, Kull, as an example to describe and validate our technique. Our model cheaply and non-intrusively estimates the load in an application at run-time, and allows for dynamic corrections to the application set up via changing the partitioning of the space between the processors (data parallelism) or adding more processors to bottleneck areas (work parallelism). We compare our estimates with actual loads observed, and propose a mechanism for incorporating the observations back into the model, making the load-balancing mechanism even more efficient.

Olga Pearce is a Ph.D. student in the Department of Computer Science at Texas A&M University working with Dr. Nancy Amato. She received her B.S. in Computer Science and Mathematics from Western Oregon University in 2004. Her research interests include parallel and distributed computing, parallel algorithms, data structures and optimizations, generic parallel libraries and tools. Her research is supported in part by an Association of Former Students Fellowship (2004-2005), a DOE GAANN Fellowship (2005-2007), and a NSF Graduate Research Fellowship (2006-2009). For more information, visit <http://parasol.tamu.edu/~olga>

2:15 PM – 3:00 PM

Jonathan Allen, LLNL

Applying computational genomics to biodefense

The availability of genome sequence data for many bacterial and viral pathogens gives new opportunity to understand the genetic basis for pathogenic function. For example, comparing two closely related microbial strains where one infects humans and the other does not, can potentially reveal important genetic pathways or mutation patterns that affect an organism's ability to impact human health. With improved understanding of dangerous pathogens, however, comes the potential for new biological threats to emerge. Computational analysis of genome sequence data gives us the opportunity to design new threat detection systems that see the world through a genomic lens. Does a sample contain genetically engineered bacteria? Could an influenza virus use a synthetic genome modeled from past pandemic strains? I will discuss some of our recent computational work to address these questions using information extracted from microbial genome data. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-407710.

Jonathan E. Allen is a Research Staff Member in the Computation division of Lawrence Livermore National Laboratory (LLNL). Dr. Allen recently completed an IC Postdoctoral Fellowship at LLNL where he worked on developing computational methods to facilitate the detection of advanced biological threats. Previously, he worked as a software engineer at The Institute for Genomic Research and developed tools for gene prediction at the University of Maryland's Institute for Advanced Computer Studies. Dr. Allen holds a Bachelors degree in Computer Science from the University of California, Santa Cruz and received his Ph.D. in Computer Science from Johns Hopkins University in 2006.

3:30 PM – 4:15 PM

Shawna Thomas, Texas A&M

From Robots to Molecules: Randomized Motion Planning for Scientific Problems

Modeling motion has a wide range of applications including robotics, computer animation, computer-aided design/virtual prototyping, computational biology, and drug design. Motion is particularly important for understanding many biochemical processes as it is often essential for function and in binding interactions. For example, several devastating neurodegenerative diseases such as Alzheimer's disease and Parkinson's disease are associated with protein misfolding and aggregation, and it has been recently shown that RNA folding kinetics can regulate gene expression and catalysis. Our understanding of molecular movement is still very limited because it is difficult to observe experimentally. Thus, computational tools are essential for studying these motions. In this talk, we describe a novel computational method for studying molecular motion based on algorithms developed in the robotics community. Our technique builds a roadmap (or graph) to model the molecule's energy landscape. From this roadmap, we can extract many (typically thousands) of folding pathways. We can also run folding simulations on the roadmap to compute global folding properties such as folding rates and

population kinetics. We have validated our technique against experimental data for both proteins and RNA. In this talk, we will focus on the protein folding application. We will show results for several small proteins and present a detailed case study of the subtle folding differences among a set of structurally similar proteins. For more information or to find our related publications, please visit our project webpage at: [http:// parasol.tamu.edu/groups/amatogroup/research/folding](http://parasol.tamu.edu/groups/amatogroup/research/folding)

Shawna Thomas is a Ph.D. candidate in the Department of Computer Science at Texas A&M University working with Dr. Nancy Amato in the Parasol Lab. She received her B.S. in Computer Engineering from Texas A&M University in 2001. Her research focus is on randomized motion planning algorithms and their application to problems in computational biology. She is also interested in the supporting areas of scientific visualization, physically-based modeling, and parallel computing. Her research is supported in part by a NSF Graduate Research Fellowship (2002-2005), a P.E.O. Scholarship (2005-2006), a DOE GAANN Fellowship (2006-2007), and an IBM Ph.D. Fellowship (2007-2009). More information about Shawna Thomas' research and publications can be found at <http://parasol.tamu.edu/~sthomas>