

Upcoming Events SC11

The SuperComputing 2011 (SC11) conference takes place this November in Seattle, Washington.

The conference continues a long and successful tradition of engaging the international community in high performance computing, networking, storage and analysis. SC11 will place an emphasis on bringing together communities to facilitate information exchange, discussions, and new collaborations for research and education related to innovating high performance computing applications and advancing scientific discovery and scholarship.



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Highlights

ORNL invention unravels mystery of protein folding



An Oak Ridge National Laboratory (ORNL) invention able to quickly predict three-dimensional structure of protein could have huge implications for drug discovery and human health.

While scientists have long studied protein structure and the mechanism of folding, this marks the first time they are able to computationally predict three-dimensional structure independent of size of the protein. Because the invention also determines possible intermediate states in the protein folding process, it provides a clearer picture and could open doors to designing new medicines for neurodegenerative diseases that are caused by incorrectly folded proteins.

Pratul Agarwal, inventor of the method and a member of the Department of Energy lab's Computer Science and Mathematics Division, believes this new method will provide benefits in many areas.

"This finding is relevant to energy, climate and health, which are all of tremendous significance today," Agarwal said. "We expect this approach to have many industrial applications through protein engineering, for example, where we expect to be able to design more efficient enzymes."

Proteins often adopt a three-dimensional structure that allows them to carry out their designated function, but such a structure has provided a computationally challenging task. Using the fundamental insights of the protein structure, dynamics and function, the ORNL invention discloses a unique computational methodology to explore the conformational energy landscape of a protein.

"One of the main advantages of this approach is that it follows the natural intrinsic dynamics of the protein and by promoting the relevant dynamical modes allows rapid exploration of the folding pathway and prediction of the protein structure," Agarwal said.

In the area of drug development, Agarwal, a computational biophysicist, expects this discovery to help in the development of treatments with little or no side effects.

Funding for this research has been provided by the National Institutes of Health, Battelle Memorial Institute, and the ORNL Laboratory Directed Research and Development program. Patent No. 7,983,887, "Fast computational methods for mechanism of protein folding and prediction of protein structure from primary sequence," was issued to Agarwal in July 2011. The technology is available for licensing.

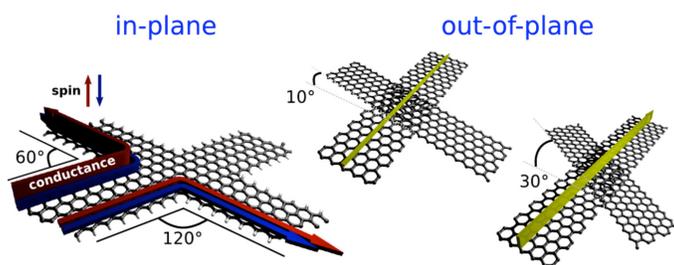
This work is reflected in two recent papers published in PLoS ONE ("Discovering conformational sub-states relevant to protein function") and The Journal of Physical Chemistry B ("Redox-Promoting Protein Motions in Rubredoxin").

Highlights (continued)

Quantum Transport in Graphene Nanonetworks

Andres R. Botello-Mendez, Eduardo Cruz-Silva, Jose M. Romo-Herrera, Florentino Lopez-Urías, Mauricio Terrones, Bobby G. Sumpter, Humberto Terrones, Jean-Christophe Charlier, and Vincent Meunier

Achievement: The quantum transport properties of graphene nanoribbon networks were investigated using first-principles calculations based on density functional theory. Both in-plane conductance in interconnected graphene nanoribbons and tunneling conductance in out-of-plane nanoribbon intersections were examined. This work demonstrates how it is possible to design ordered graphene nanoribbon networks capable of efficiently guiding electrons along desired and predetermined paths. In addition, certain graphene intersections exhibit different transmission probability for spin up and spin down electrons, indicating possible applications as spin filters.



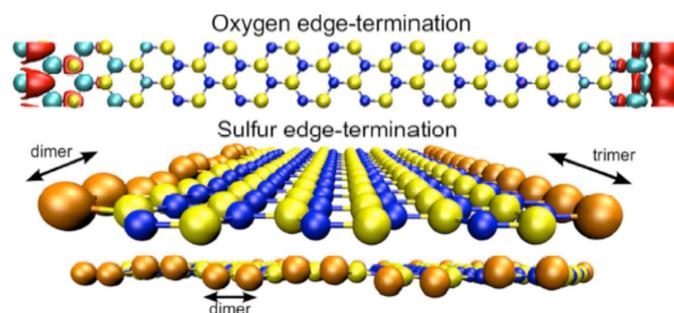
Significance: It is now well-known that graphene exhibits remarkable electronic properties such as record-high electronic mobilities, can support large current densities, and exhibits exceptionally high thermal conductivity. These properties make graphene one of the most attractive materials for electronic applications. However, to be introduced as a material for mainstream logic electronic devices, a bandgap must be induced; for example, by structural alterations of the two-dimensional (2D) graphene sheet that effectively reduces the system's dimensionality and leads to one-dimensional (1D) graphene nanoribbons (GNRs). Nano-circuits or networks constructed from these 1D systems can be constructed, but little was known regarding their physicochemical properties as a function of the architecture. Clearly it would be expected that the resulting assemblies possess mechanical, electronic, and porosity properties that are strikingly different from those of the isolated 1D blocks. Our work defines how quantum transport properties depend on the intersection angles between in-plane and out-of-plane GNRs, thereby, providing supramolecular design rules for successfully building networks for guiding electrons along desired and predetermined paths. Additionally, certain graphene intersections exhibit different transmission probability for spin up and spin down electrons, suggesting the possible applications as spin filters.

Credit – This work is published in Nano Letters. The research at Oak Ridge National Laboratory was performed at the Center for Nanophase Materials Sciences, sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy and utilized computational resources from the National Center for Computational Sciences.

Boron Nitride Nanoribbons Become Metallic

Alejandro Lopez-Bezanilla,, Jingsong Huang, Humberto Terrones, and Bobby G. Sumpter

Achievement: Boron Nitride (BN) is a layered material consisting of one-atom-thick BN sheets that bear close resemblance to graphene but differ by a remarkable ionic character. Consequently, unlike graphene, which is a semimetal with superb electron mobility, unpassivated BN is a wide bandgap insulator. In this work, we show how to close the electronic gap of BN-based materials, rendering them metallic. This is accomplished by using first-principles calculations to show how oxygen (O) and sulfur (S) functionalizations of zigzag boron nitride nanoribbons (zBNNRs) lead to quasi-1D metallic conductors. The work highlights widely tunable zBNNRs electronic and magnetic properties, illustrating the feasibility of BN-based materials for providing new opportunities towards enabling nanoelectronic devices.



Significance: O and S functionalized zBNNRs exhibit drastically different properties from the semiconducting and nonmagnetic H edge-terminated zBNNRs. In addition to being metallic, O edge-terminated zBNNRs have two energetically degenerate magnetic ground states with a ferrimagnetic character on the B edge. In contrast, S edge-terminated zBNNRs are nonmagnetic but still metallic. A second type of functionalization with O or S atoms embedded in the center of zBNNRs forming a nanowire yields semiconducting nanoribbons. The various BN materials analyzed share a common feature: functionalizing atoms create extended nanowires along the principle axis of the zBNNRs with charge densities at the vicinity of Fermi level localized either on the ribbon edge in the case of edge termination, or within a narrow area across the ribbon width in the case of atom lines joining two zBNNRs. Due to the localized character of these nanowire “defects,” the results can be extrapolated to arbitrarily large zBNNRs without loss of generality. Experimentally, the functionalization of zBNNRs may be realized, e. g., by applying oxygen plasma on the edges of BN ribbons obtained by unzipping BN nanotubes. Therefore, this work illustrates the feasibility of using BN materials as suitable candidates for the nanoelectronics field.

Credit – This work is published in Nano Letters. The research was performed at Oak Ridge National Laboratory's Center for Nanophase Materials Sciences, sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy and utilized computational resources from the National Center for Computational Sciences.

Awards

Distinguished Employee Program

The Computing and Computational Sciences Directorate program is recognizing an employee from each division each month for distinguished contributions; the first awards were made in April, 2011.

George Fann (July)

George Fann initiated, derived, and developed many of the mathematical results and numerical methods in Multiresolution Adaptive Numerical Environment for Scientific Simulation (MADNESS) that recently won an R&D 100 award. He also co-developed and prototyped the numerical methods for solving singular and pseudo-differential operators in applications in collaboration with Professor Gregory Beylkin at the University of Colorado at Boulder and Professor Robert Harrison of Joint Institute for Computational Sciences (JICS). He continues to derive and prototype new computational methods and scalable numerical algorithms. He was also an instrumental player in the application of MADNESS to computational chemistry (with Professor Robert Harrison) and nuclear physics (with Dr. Witold Nazarewicz in the Physics Division). He continues to be a principal investigator and a collaborator of numerous projects to further develop and enhance the algorithmic and mathematical capabilities of MADNESS and its applications to other disciplines.

MADNESS is a free open-source general purpose user-friendly numerical framework and software for the development scientific simulations from laptops to massively parallel supercomputers. MADNESS utilizes the latest parallel computing and solution methodologies to solve many dimensional integral and differential equations accurately and precisely for real-world problems. MADNESS provides a new platform for scientists and engineers to easily create new applications with assurance in the exactness of their results.

Collin McCurdy (August)

Collin McCurdy developed Memphis - a tool for pinpointing memory-related performance problems in multi-threaded applications. Collin has used Memphis to optimize several important DOE applications, and has had those optimizations integrated into several applications. For example, with Memphis, this work led to a ~25% performance improvement of the XGC1 fusion application at scale on Jaguar. DOE ASCR funds Memphis, and this is joint work with Patrick Worley, Don Maxwell, and Jeffrey Vetter.

Terry Jones (September)

As part of ASCR funded research, Terry Jones worked to develop I/O forwarding capabilities for the Cray. Terry also worked with the Technical University of Dresden and NCCS, in the context of the OLCF-3 project, to incorporate the I/O forwarding capabilities into the Vampir performance analysis tool suite. With these new capabilities, trace-based performance analysis was performed on an application sized at about 200,000 processes, which is an order of magnitude increase in the job size for which such analysis is feasible. This work is helping the OLCF meet its goal of being able to analyze full user applications at system scale.

Other Awards/Recognition

Pratul Agarwal

CSMD Researcher Pratul Agarwal has been awarded a patent for his invention "Fast Computational Methods for Predicting Protein Structure from Primary Amino Acid Sequence."

According to the US Patent Office, "the invention provides a method utilizing primary amino acid sequence of a protein, energy minimization, molecular dynamics and protein vibrational modes to predict three-dimensional structure of a protein."

David Erickson

David Erickson was named a Joint 'Full' Professor between the Department of Civil and Environmental Engineering, University of Tennessee, Knoxville and ORNL in FY2011.

Moving On

Edoardo Aprà

Edo has returned to PNNL to continue his work with developing and maintaining NWChem.

HPCwire's recipient of the 2010 HPCwire Reader's Choice Award for Supercomputing Achievement, Dr. Aprà was honored for his work with a computational chemistry application known as NWChem, which was developed at Pacific Northwest National Laboratory. Under Aprà's expert guidance, the application reached an astounding 1.39 thousand trillion calculations per second, or 1.39 petaflops, on Oak Ridge National Laboratory's (ORNL) Jaguar system. Previously, the same team led by Aprà was a finalist for the prestigious Gordon Bell Prize in 2009, which recognizes the world's top supercomputing application.

Phani Nukala

Phani has left ORNL to be a Senior Quantitative Strategist at Graham Capital Management. Graham Capital Management is a \$9B hedge fund that employs a diversified approach to investing including multi-strategy, discretionary, quantitative, global macro, relative value, equity long/short, and arbitrage strategies as hedging techniques while making investments. His role will be to develop quantitative strategies for portfolio and risk management.

At ORNL, Dr. Nukala's research interests were in the broad areas of computational mechanics and materials science, numerical analysis, statistical physics, multiscale methods, bio-inspired materials, game theory, and high-performance scientific computing. For advancement of science and technology and demonstrated leadership throughout his professional career, Dr. Nukala received twelve awards over the years including the Emeralds Award from Science Spectrum Magazine. He holds two patents, and published more than fifty refereed journal publications and thirteen refereed conference proceedings.

Vinod Tipparaju

Vinod Tipparaju departed from ORNL on August 26th for a new position at AMD. Vinod was a key contributor to programming models activities that included MPI-3, Global Arrays, and NWChem. Vinod also contributed to many publications and was a Gordon Bell finalist at SC09. At AMD, Vinod will develop system software for AMD's Fusion system.

Community Service

Christian Engelmann served as program chair and session chair of the 4th Workshop on Resiliency in High Performance Computing (Resilience) in Clusters, Clouds.

David Erickson served as a member of the Program Committee for the 5th International Workshop on Knowledge Discovery from Sensor Data (SensorKDD-2011), San Diego, CA, August 21, 2011.

David Erickson has been appointed a Member, HPC Advisory Panel to National Center for Atmospheric Research (NCAR) Computational and Information Systems Laboratory (CISL) for a 3 year term starting in Fall 2011.

Eirik Endeve has been serving as the astrophysics representative on the OLCF User Council.

Eirik Endeve served as a session chair for the session on Plasma, Turbulence at the Turbulent Mixing and Beyond 2011 (TMB2011) conference in Trieste, Italy.

Anthony Mezzacappa served on the Organizing Committee for the Conference on Computational Physics 2011 (CCP2011).

Anthony Mezzacappa served on the Editorial Board for the Journal *Computational Science and Discovery*.

Anthony Mezzacappa served on the Editorial Board for the *International Journal of High Performance Computing Applications*.

George Ostrouchov served as a member of the Program Committee for the 5th International Workshop on Knowledge Discovery from Sensor Data (SensorKDD-2011), August 21-24, 2011, San Diego, CA.

George Ostrouchov served as a member of the Program Committee for the 4th International Workshop on Resiliency in High Performance Computing, August 29 – September 2, 2011, Bordeaux, France.

Community Service (continued)

Line Pouchard served as the co-chair and co-organizer of the First Linked Science Workshop at the International Semantic Web Conference, October 23-27, 2011, Bonn.

Phil Roth served on the committee for the Parallel Software Tools and Tool Infrastructures (PSTI) workshop.

Stephen Scott served as director of HPCVirt and Resilience workshops.

Bobby Sumpter was the conference organizer and session chair for the workshop "Materials by Design," Oak Ridge, TN September 21-22 (2011).

Bobby Sumpter was the conference organizer and session chair for the workshop "Sustainable Energy Future: Nanomaterials Enabled Photovoltaics," Oak Ridge, TN September 22-23, 2011.

Jeffrey Vetter served on the Program Committee for PPOPP 2012 Program Committee.

Jeffrey Vetter served on the Organizing Committee for SciDAC 2011 Organizing Committee.

Jeffrey Vetter served on the Tutorials Committee for SuperComputing 2011.

Patrick Worley was a co-organizer of the Software Engineering Working Group meeting at the 16th Annual Community Earth System Model Workshop, June 23, 2011.

New Faces in CSMD



Anne Calhoun

Computational Earth Sciences
Group Administrative Assistant



Billy Fields

Computational Chemical and Materials Sciences
Computational Mathematics
Statistics and Data Science
Group Administrative Assistant



Ben Mayer

Computational Earth Sciences
R&D Associate/Software Engineer

Ben's specialties are High Performance Parallel Computing, Optimization, and Data Mining



Matt Reuter

Computational Chemical and Materials Sciences
Wigner Fellow

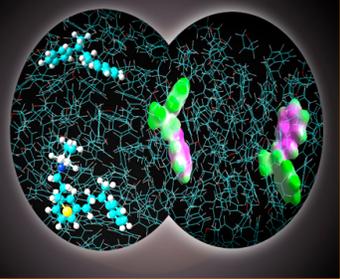
Matt's specialties are Electron Transport in nanoscale systems and algorithm development.

Publications/Presentations

Publications

Journal Publications

- Jose Alonzo, Jihua Chen, Jamie Messman, Xiang Yu, Kunlun Hong, SuxiangDeng, Onome Swader, Mark Dadmun, John F. Ankner, Phillip Britt, Jimmy W. Mays, Massimo Malagoli, Bobby G. Sumpter, Jean-Luc Brédas, S. Michael Kilbey II, Assembly and Characterization of Well Defined High Molecular Weight Poly(p-phenylene) Polymer Brushes, *Chemistry of Materials*, (in press 2011).
- “Simple impurity embedded in a spherical jellium: Approximations of density functional theory compared to quantum Monte Carlo benchmarks.” M. Bajdich, P. R. C. Kent, J. Kim, F. A. Reboredo. *Physical Review B* 84 075131 (2011).
- José Ramón Blas, Oscar Huertas, Carolina Tabares, Bobby G. Sumpter, Miguel Fuentes-Cabrera, Modesto Orozco, Pablo Ordejón, F. Javier Luque, Structural, Dynamical and Electronic Transport Properties of Modified DNA Duplexes Containing Size-Expanded Nucleobases, *J. Phys. Chem. B*. DOI: [10.1021/jp205122c](https://doi.org/10.1021/jp205122c) (2011).
- J. Dennis, J. Edwards, K. J. Evans, O. Guba, P.H. Lauritzen, A. Mirin, A. St.-Cyr, M. Taylor, P. Worley (2011). CAM-SE: A scalable spectral element dynamical core for the Community Atmosphere Model. *Int. J. High Perf. Comp.*, accepted for publication.
- J. M. Dennis, J. Edwards, K. J. Evans, O. Guba, P. H. Lauritzen, A. A. Mirin, A. St-Cyr, M. A. Taylor, and P. H. Worley, CAM-SE: A scalable spectral element dynamical core for the Community Atmosphere Model, *International Journal for High Performance Computer Applications*. (accepted)
- J. M. Dennis, M. Vertenstein, P. H. Worley, A. A. Mirin, A. P. Craig, R. Jacob, and S. A. Mickelson, Computational Performance of Ultra-High-Resolution Capability in the Community Earth System Model, *International Journal for High Performance Computer Applications*. (accepted)
- Guang Feng, Jingsong Huang, Bobby G. Sumpter, Vincent Meunier, Rui Qiao, “A counter-charge layer in generalized solvents” framework for electrical double layers in neat and hybrid ionic liquid electrolytes, *Phys. Chem. Chem. Phys.* 13, 14723-14734 (2011).
- “Formation, characterization and dynamics of onion like carbon structures from nanodiamonds using reactive force-fields for electrical energy storage.” P. Ganesh, P. R. C. Kent, and V. Mochalin. Accepted in *Journal of Applied Physics* (2011).
- P. R. Gent, G. Danabasoglu, L. J. Donner, M. M. Holland, E. C. Hunke, S. R. Jayne, D. M. Lawrence, R. B. Neale, P. J. Rasch, M. Vertenstein, P. H. Worley, Z-L Yang, and M. Zhang, The Community Climate System Model Version 4, *Journal of Climate*. (accepted)
- A. Knebe et al., (36 authors), "Haloes gone MAD: The Halo-Finder Comparison Project." *Monthly Notices of the Royal Astronomical Society* 415(3):2293--2318, August 2011.
- S. Maiti, M.M. Korshunov, T.A. Maier, P.J. Hirschfeld, and A.V. Chubukov, “Evolution of superconductivity in iron---based systems with doping,” accepted for publication in *Phys. Rev. Lett.* (2011).
- J. Meredith, P. Roth, K. Spafford, and J.S. Vetter, "Performance Implications of Non-Uniform Device Topologies in Scalable Heterogeneous GPU Systems," in *IEEE Micro* (special issue on CPU, GPU, and Hybrid Computing), vol. 99, 2011.
- J. Messman, D. Pickel, D. Uhrig, B. G. Sumpter, M. Goswami, and J. Mays, Combating Ionic Aggregation using Dielectric Forces- Combining Modeling/Simulation and Experimental Results to Explain End-capping of primary Amine Functionalized Polystyrene, *Polymer Chemistry* (in press 2011) [Cover of the Journal].



Cover Art

The image above will appear on the upcoming cover of the journal *Polymer Chemistry*. It is from Bobby Sumpter's paper "Combating Ionic Aggregation using Dielectric Forces- Combining Modeling/ Simulation and Experimental Results to Explain End-capping of primary Amine Functionalized Polystyrene."

Publications/Presentations (continued)

- K. Spafford, J. Meredith, and J.S. Vetter, "Quartile and Outlier Detection on Heterogeneous Clusters Using Distributed Radix Sort," in Workshop on Parallel Programming on Accelerator Clusters (PPAC 2011). Austin, TX, USA: IEEE, 2011.
- Say-Lee Teh, Dias Linton, Bobby Sumpter, and Mark D. Dadmun, Controlling Non-Covalent Interactions to Modulate the Dispersion of Fullerenes in Polymer Nanocomposites, *Macromolecules* DOI: [10.1021/ma200795g](https://doi.org/10.1021/ma200795g) (2011).
- J.S. Vetter, R. Glassbrook, J. Dongarra, K. Schwan, B. Loftis, S. McNally, J. Meredith, J. Rogers, P. Roth, K. Spafford, and S. Yalamanchili, "Keeneland: Bringing Heterogeneous GPU Computing to the Computational Science Community," *IEEE Computing in Science and Engineering* 13(5):90-5, 2011.
- Xiaojun Wang, Kunlun Hong, Durairaj Baskaran, Monojoy Goswami, Bobby Sumpter, Jimmy Mays, Asymmetrical Self-assembly From Fluorinated and Sulfonated Block Copolymers in Aqueous Media, *Soft Matter Commun.* 7, 7960-7964 (2011). [Most downloaded ASAP article]
- J. Woodring, K. Heitmann, J. Ahrens, P. Fasel, C. Hsu, S. Habib, and A. Pope, "Analyzing and Visualizing Cosmological Simulations with ParaView." *The Astrophysical Journal Supplement Series*, 195(1):11, July 2011.
- C. Zhang, M. Wang, H. Luo, M. Wang, M. Liu, J. Zhao, D.L. Abernathy, T. A. Maier, K. Marty, M.D. Lumsden, S. Chi, S. Chang, J.A. Rodriguez-Rivera, J.W. Lynn, T. Xiang, J. Hu, P. Dai, "Neutron Scattering Studies of spin excitations in hole-doped Ba_{0.67}K_{0.33}Fe₂As₂ superconductor," accepted for publication in *Nature Scientific Reports* (2011).
- "Anomalous Lattice Dynamics near Ferroelectric Instability in PbTe." Y. Zhang, X. Ke, P. R. C. Kent, C. Chen, and J. Yang. Accepted in *Physical Review Letters* (2011).
- "Nanodopant-induced band modulation in AgPbmSbTe₂+m-type thermoelectrics." Y. Zhang, X. Ke, C. Chen, J. Yang, and P. R. C. Kent. *Physical Review Letters* 106 206601 (2011).
- Zhenzhong Sun, Kai Xiao, Xiang Yu, Kunlun Hong, Jong Kahk Keum, Jim Browning, Ilia N. Ivanov, Jihua Chen, Jose Alonzo, Dawen Li, Bobby Sumpter, Andrew Payzant, Christopher Rouleau, David B. Geohegan, P3HT-b-PS Copolymers as P3HT/PCBM Interfacial Compatibilizers for High Efficiency Photovoltaics, *Adv. Mat.* (in press, 2011).

Book Chapters

- Jingsong Huang, Ariana Beste, Jarod Younker, Alvaro Vazquez-Mayagoitia, Eduardo Cruz-Silva, Miguel Fuentes-Cabrera, Jacek Jakowski, Alejandro Lopez-Bezanilla, Vincent Meunier, and Bobby G. Sumpter, "Advancing Understanding and Design of Functional Materials through Theoretical and Computational Chemical Physics," Springer, 2011 (in press).
- Alejandro Lopez-Bezanilla, Stephan Roche, Eduardo Cruz-Silva, Bobby G. Sumpter, and Vincent Meunier, "Electronic Transport in Carbon Nanomaterials," *Encyclopedia of Nanoscience and Nanotechnology*, Springer (2011).
- N. S. V. Rao, Measurement-based statistical fusion methods for distributed sensor networks, in *Distributed Sensor Networks*, 2nd Edition, R. R. Brooks and S. S. Iyengar (editors), 2011, Chapman and Hall Publishers.
- P. H. Worley, M. Vertenstein, and A. Craig, Community Climate System Model, in *Encyclopedia of Parallel Computing*, ed. D. Padua, Springer, 2011.
- M. Zhu, R.R. Brooks, S. Ding, Q. Wu, N. S. V. Rao, S.S. Iyengar, Chebyshev's inequality-based multisensor data fusion in self-organizing sensor networks, in *Distributed Sensor Networks*, 2nd Edition, R. R. Brooks and S. S. Iyengar (editors), 2011, Chapman and Hall Publishers.

Conference Papers/Abstracts:

- K. Brigham, B. V. K. Vijay Kumar, and N. S. V. Rao, Robust fusion algorithms for state estimation over long-haul networks, 14th ONR/GTRI Workshop on Target Tracking and Sensor Fusion, 2011, abstract.
- J. C. Chin, D. K. Y. Yau, and N. S. V. Rao, Efficient and robust localization of multiple radiation sources in complex environments, International Conference on Distributed Computing Systems, 2011.
- Erickson, D. J. III, United Nations Environment Program (UNEP), Invited author for effects section on "Increased UVB fluxes and global biogeochemical cycle interaction with climate change," Basel, Switzerland, Aug. 24-Sep. 1, 2011.
- Y. Gu, Q. Wu, and N. S. V. Rao, Analyzing execution dynamics of scientific workflows for latency minimization in resource sharing environments, Workshop on Scientific Workflows, 2011.

Publications/Presentations (continued)

- Oscar Hernandez, Wei Ding, Barbara Chapman, Christos Kartsaklis, Ramanan Sankaran, and Richard Graham. Experiences with High-Level Programming Directives for Porting Applications to GPUs. In Proceedings of Facing the Multicore-Challenge II Conference. Karlsruhe Institute of Technology. September 2011 (Accepted, to appear in proceedings).
- C. Hsu and S. Poole, "Power Measurement for High Performance Computing: State of the Art." International Workshop on Power Measurement and Profiling (PMP), July 2011. Orlando, FL.
- R. Kumar, and B. G. Sumpter, "Quantitative analysis of chain packing in polymer melts using large scale molecular dynamics simulations," Proc. SciDac 2011.
- E.J. Lingerfelt, O.E.B. Messer, J.A. Osborne, R.D. Budiardja, and A. Mezzacappa, A Multitier System for the Verification, Visualization and Management of CHIMERA, Procedia Computer Science, Vol 4, Proceedings of the International Conference on Computational Science 2011, Pages 2076-2085.
- Q. Liu, X. Wang, and N. S. V. Rao, Selective fusion of state estimates under random delays and loss in long-haul sensor networks, 14th ONR/GTRI Workshop on Target Tracking and Sensor Fusion, 2011, abstract.
- A. Lopez-Benzanilla, J. S. Huang, H. Terrones, and B. G. Sumpter, "Electronic Structure Calculations on Edge-functionalized Armchair Boron Nitride Nanoribbons," Proc. SciDac 2011.
- C. Y. T. Ma, N. S. V. Rao, and D. K. Y. Yau, A game-theoretic study of attack and defense in cyber-physical systems, International Workshop on Cyber-Physical Networking Systems, 2011.
- N. S. V. Rao, Localization-Based detection under network losses, International Conference on Information Fusion, 2011.
- N. S. V. Rao, B. V. K. Vijay Kumar, K. Brigham, and X. Wang, Effects of computing and communications on state fusion over long-haul sensor networks, 14th ONR/GTRI Workshop on Target Tracking and Sensor Fusion, 2011, abstract.
- R. Sisneros, J. Huang, G. Ostrouchov, and F. Hoffman (2011). Visualizing Life Zone Boundary Sensitivities Across Climate Models and Temporal Spans, Procedia Computer Science, Vol. 4, p.1582-1591.
- N. S. V. Rao, C. Y. T. Ma, and D. K. Y. Yau, On robustness of a class of cyber-physical network infrastructures, Workshop on Design, Modeling and Evaluation of Cyber Physical Systems, 2011.
- Bradley W. Settlemyer, Nageswara Rao, Stephen W. Poole, Stephen W. Hodson, Susan Hicks, and Paul Newman. "Experimental Analysis of 10Gbps Transfers Over Physical and Emulated Dedicated Connections." International Conference on Computing, Networking and Communications (ICNC 2012), Maui, Hawaii, USA.

Presentations

Invited Presentations

- Billings, Jay Jay (ORNL), "HPC Updates to Scale for Cross Section Processing"
- Das, Debasish (ORNL), Steinhäuser, Karsten J K(ORNL), Kao, Shih-Chieh (ORNL), Ganguly, Auroop R(ORNL), Branstetter, Marcia L(ORNL), Erickson III, David J(ORNL), Flanery, Raymond (Oak Ridge National Laboratory (ORNL)), Gonzalez, Maria Martinez(Oak Ridge National Laboratory (ORNL)), Hays, Cynthia (University of Nebraska, Lincoln), King, Anthony Wayne(ORNL), Lenhardt, W Christopher(ORNL), Oglesby, Robert J(ORNL), Patton, Robert M(ORNL), Rowe, Clinton (University of Nebraska, Lincoln), Sorokine, Alexandre (ORNL), Steed, Chad A(ORNL), "Uncertainty and extremes analysis to evaluate dynamical downscaling of climate models," AGU Fall Meeting
- Elliott, Scott (Los Alamos National Laboratory), Erickson III, David J (ORNL), Mirin, Art (Lawrence Livermore National Laboratory), Jacob, Robert L.(Argonne National Laboratory), "Earth System Modeling of Ozone, Methane, and DMS," AGU Fall Meeting
- Endeve, Eirik, International Congress on Industrial and Applied Mathematics 2011 (ICIAM2011), Vancouver, Canada, July 22, in mini-symposium on advanced numerical methods for kinetic simulations and their applications, Numerical Methods for Neutrino Kinetics in Core Collapse Supernova Models
- Endeve, Eirik, Turbulent Mixing and Beyond 2011 (TMB2011), Trieste, Italy, August 25, 2011 Magnetic Field Amplification from Turbulent Flows in Core-Collapse Supernovae

Publications/Presentations (continued)

- Erickson III, David J. (ORNL), Fernandez, Steven J. (ORNL), Branstetter, Marcia L. (ORNL), Butler, George (University of Tennessee, Knoxville (UTK) & Oak Ridge National Laboratory (ORNL)), Ganguly, Auroop R. (ORNL), Oglesby, Robert J. (ORNL), Steinhäuser, Karsten J. K. (ORNL), Kodra, Evan A. (ORNL), "Climate Impacts on US Energy Infrastructure: A New High Resolution Model, Policy Implications and Feedbacks," AGU Fall Meeting.
- Erickson, David J. (ORNL), "Monthly Anthropogenic CO₂ fluxes: Impacts on the atmospheric CO₂ seasonal cycle and implications for models of the terrestrial biosphere," AGU Fall Meeting.
- Erickson, D. J. III, "Data mining, exa-scale workflow and financially germane carbon/climate weather," Invited Lecture, The First Workshop on Understanding Climate Change from Data (NSF), University of Minnesota, Minneapolis, MN, Aug.15-16, 2011.
- Erickson, D. J. III, Invited Keynote Speaker, Gordon Research Conference, Sustainability and the role of visualization, Visualization in Science and Education, Transformation by visualization: Radical effects on Learning in Sciences and Across Education, "Global climate change, sustainability and visualization of atmospheric CO₂," Bryant University, Smithfield, R. I., July 13-17, 2011.
- Erickson, D. J. III, Invited lecture, Climate-Energy Modeling, Presentation to Dr. Rick Duke, Bob Marlay et al., Office of Climate Change Policy and Technology, Department of Energy, Oak Ridge National Laboratory, Oak Ridge, TN, Aug. 24, 2011.
- Erickson, D. J. III, Invited Keynote Lecture, Eawag-UNEP Symposium: Stratospheric ozone depletion, solar UV radiation and climate change: Interactive effects and feedbacks, Forum Chriesbach, C20, Eawag Dubendorf, Switzerland, Aug. 30, 2011.
- Erickson III, David J(ORNL), "Earth system modeling beyond the peta-scale."
- Erickson III, David J(ORNL), "Constraining the terrestrial biosphere CO₂ fluxes via anthropogenic CO₂ emission seasonality."
- Erickson III, David J(ORNL), "Stratospheric ozone depletion, solar UV radiation and climate change: Interactive effects and feedbacks," Eawag-UNEP Symposium
- Erickson III, David J(ORNL), "Climate-Energy Modeling"
- Erickson III, David J(ORNL), "Knowledge Discovery from Sensor Data (SensorKDD-2011)," 5th International Workshop on Knowledge Discovery from Sensor Data (SensorKDD-2011).
- Erickson III, David J(ORNL), "Global climate change, sustainability and visualization of atmospheric CO₂," Gordon Research Conference, Sustainability and the role of visualization, Visualization in Science and Education, Transformation by visualization: Radical effects on Learning in Sciences and Across Education.
- Erickson III, David J(ORNL), "Increased UVB fluxes and global biogeochemical cycle interaction with climate change."
- Erickson III, David J(ORNL), Andres, Robert Joseph(ORNL), Hoffman, Forrest (ORNL), Branstetter, Marcia L(ORNL), Long, Michael S(ORNL), Allen, Melissa R(ORNL), "Fossil fuel seasonality impacts on atmospheric CO₂ concentrations," CESM Workshop
- Erickson, David J(ORNL), "Atmospheric CO₂ simulations using GEOS-5: Data assimilation, data fusion and treaty verification," A-Train Symposium
- Erickson III, David J(ORNL), "Paleometeorology: High resolution Northern Hemisphere wintertime mid-latitude dynamics during the last glacial maximum," AGU Fall Meeting
- Climate Forum Plenary Speaker: K. Evans, "Design and analysis of the Community Earth System Model," Developing International Geoscientific Conference, University of Tennessee, Knoxville, TN, Sept., 2011.
- "Challenges in Modeling the Global Earth System," ICIS Workshop on Multiphysics Simulations: Challenges and Opportunities, Park City, UT, USA. July 31–Aug 6, 2011. K. Evans
- "Progress towards high-resolution continental-scale ice sheet simulations using a higher-order dynamical core in Glimmer-CISM," K.J. Evans, Community Earth System Model Workshop, Breckenridge, CO, June, 2011.

Publications/Presentations (continued)

- "Using Computational Science to Model the Earth's Climate," K. Evans, Harnessed Atom Curriculum Program, Oak Ridge Institute for Research and Education through the Dept. of Nuclear Energy, Oak Ridge, TN, July 2011.
- Hauck, Cory D, "A Realizability-Preserving, Discontinuous Galerkin Scheme for the S_M Model of Radiative Transfer," UTK, Sept. 26, 2011
- Hauck, Cory D(ORNL), "Optimization-Based Moment Closures in Kinetic Theory and Transport"
- Paul Kent, "Challenges of first principles calculations for Lithium-Ion Batteries and Structural Materials," Invited talk, SciDAC 2011 Meeting, July 2011, Denver, CO.
- King, Anthony Wayne(ORNL), Ganguly, Auroop R(ORNL), Erickson III, David J(ORNL), Lenhardt, W Christopher(ORNL), "Climate science support for the 2010 Quadrennial Defense Review (QDR): Projection and analysis of climate change impacts on defense interests," Symposium on Environment, Energy, and Sustainability, NDIA
- Joshua Ladd, Manjunath Gorentla Venkata, Richard Graham, Pavel Shamis, "Analyzing the Effects of Multicore Architectures and On-host Communication Characteristics on Collective Communications," accepted the SRMPDS workshop in conjunction with ICPP
- Thomas Maier, "How does the Hubbard Model guide us in the search for higher-Tc superconductors?," Condensed Matter seminar, University of Florida, Gainesville, Sept. 2011.
- Thomas Maier, "Superconductivity in cuprate, organic and iron-based materials: A dynamic cluster quantum Monte Carlo perspective," Electronic structure of novel materials conference, Tegernsee, Germany, Sept. 2011.
- Thomas Maier, "Computational Insight into High-Temperature Superconductivity," Annual Research Meeting of the Office of Science Graduate Fellowship Program, ORNL, July 2011.
- Thomas Maier, "Superconductivity in Striped and Multi-Fermi-Surface Hubbard Models: From the Cuprates to the Pnictides," Stripes 2011 Conference, Rome, Italy, July 2011.
- Ostrouchov, George (ORNL), "R Programming Language Workshop"
- Rowe, Clinton (University of Nebraska, Lincoln), Oglesby, Robert J(ORNL), Erickson III, David J(ORNL), "Resolving the Effects of Complex Topography on Regional Climate and Climate Change: The Need for Very High Spatial Resolution," AGU Fall Meeting
- Sullivan, Blair, "Are Tree Decompositions Practical for Large Scale Computing?," ICIAM 2011, Vancouver, BC, July 21, 2011; joint work w/ Chris Groer
- Sullivan, Blair, "Solving Large Graph Problems Using Tree Decompositions: A Computational Study," Virginia Tech, Blacksburg, VA, Sept. 7, 2011; joint work w/Chris Groer, Dinesh Weerapugge.
- Worley, Patrick H(ORNL), "A Scalable and Extensible Earth System Model."
- Worley, Patrick H(ORNL), Mirin, Arthur A.(Lawrence Livermore National Laboratory (LLNL)), "Performance Engineering of the Community Climate System Model."
- Worley, Patrick H(ORNL), "SciDAC Update," 16th Annual CESM Workshop
- Worley, Patrick, Gemini Performance Evaluation: status report Cray - Sandia National Laboratories XE6 Workshop, Computer Science Research Institute Albuquerque, NM, September 28, 2011.
- Zhang, Xiaoguang (ORNL), "New Directions in Spintronics: Organic Spintronics and Giant Coulomb Blockade Magnetoresistance"

Presentations

- Baker, Christopher G(ORNL), "Gradually transitioning library users to the hybrid-parallel paradigm," ICIAM 2011 -- 7th International Congress on Industrial and Applied Mathematics.
- Bell, Zane W. (ORNL), Davidson, Gregory G. (ORNL), D'Azevedo, Ed F. (ORNL), Evans, Thomas M. (ORNL), Joubert, Wayne (ORNL), Munro Jr, John K. (ORNL), and Patlolla, Dilip Reddy (ORNL), "Python for Development of OpenMP and CUDA Kernels for Multidimensional Data (presentation)," 2011 Symposium on Application Accelerators in High Performance Computing (SAAHPC'11)

Publications/Presentations (continued)

- Branstetter, Marcia L. (ORNL), Erickson III, David J. (ORNL), Jacob, Robert L. (Argonne National Laboratory), Elliott, Scott (Los Alamos National Laboratory), "Analysis of DMS and SO₄ in a coupled chemistry-climate simulation using CCSM: Using optical depth and radiative forcing proxies," CESM Workshop.
- Budiardja, R., Endeve, E., Cardall, C., and Mezzacappa, A., "Exploring the generation of magnetic fields by the stationary accretion shock instability with GenASiS," American Astronomical Society, AAS Meeting #217, #410.02; Bulletin of the American Astronomical Society, Vol 43, 2011.
- Camacho Bonaparte, Yael M(ORNL), Ostrouchov, George (ORNL), Sisneros, Roberto R(ORNL), and Kettani, Houssain (ORNL), "Preprocessing climate data for access to local spatial extremes," ORAU Summer 2011 Student Poster Session
- Colon, Javier (ORNL), Ostrouchov, George (ORNL), and Kettani, Houssain (ORNL), "Extracting features from climate data using VisIt," ORAU Summer 2011 Student Poster Session
- Craig, Anthony (National Center for Atmospheric Research (NCAR)), Mirin, Arthur A.(Lawrence Livermore National Laboratory (LLNL)), Taylor, Mark (Sandia National Laboratories (SNL)), Worley, Patrick H(ORNL), "Computer Performance of the Community Earth System Model," 16th Annual CESM Workshop
- Endeve, E., Cardall, C., Budiardja, R., Beck, S., Bejnood, A., and Mezzacappa "Magnetic field evolution in three-dimensional simulations of the stationary accretion shock instability," A., American Astronomical Society, AAS Meeting #217, #337.23; Bulletin of the American Astronomical Society, Vol 43, 2011.
- Hauck, Cory D(ORNL), "Topics in Kinetic Simulation: Introduction and Reduced-Order Modeling," 2011 International Congress on Industrial and Applied Mathematics.
- Humble, T. S. "GNU Radio for Quantum Optical Communication," GNU Radio Conference, Philadelphia, PA (Sept 2011)
- Joshua Hursey, Jeffrey M. Squyres, and Terry Dontje. Locality-aware parallel process mapping for multi-core HPC systems. In IEEE International Conference on Cluster Computing, Austin, TX, September 2011. (Poster).
- Joshua Hursey, Thomas Naughton, Geoffroy Vallee, and Richard L. Graham. A log-scaling fault tolerant agreement algorithm for a fault tolerant MPI. In EuroMPI 2011: Proceedings of the 18th EuroMPI Conference, Santorini, Greece, September 2011.
- Joshua Hursey, Richard L. Graham, Greg Bronevetsky, Darius Buntinas, Howard Pritchard, and David G. Solt. Run-through stabilization: An MPI proposal for process fault tolerance. In EuroMPI 2011: Proceedings of the 18th EuroMPI Conference, Santorini, Greece, September 2011. (Poster).
- Joshua Hursey. A Log-Scaling Fault Tolerant Agreement Algorithm for a Fault Tolerant MPI, Oak Ridge National Laboratory CSMD Seminar, August 2011.
- Kulkarni, Nagraj S(ORNL), Radhakrishnan, Balasubramaniam (ORNL), Todd, Peter J(ORNL), Sohn, Yong Ho (University of Central Florida), Brennan, Sarah (University of Central Florida), Coffey, Kevin (University of Central Florida), Hunter Jr., Jerry (Virginia Polytechnic Institute and State University (Virginia Tech)), "Tracer Diffusion Databases for ICME," 1st World Congress on Integrated Computational Materials Engineering.
- Lingerfelt, E., "Developing Multitier Software Applications for Astrophysics, Cosmology and Nuclear Physics at ORNL," Seminar, East Tennessee State University, Department of Physics and Astronomy, April 2011.
- Odbadrakh, Khorgolkhuu (ORNL), Rusanu, Aurelian (ORNL), Stocks, George Malcolm(ORNL), Samolyuk, German D (ORNL), Wang, Yang (Pittsburgh Supercomputing Center), Nicholson, Don M(ORNL), "Large Scale Density Functional Theory Modeling of Magnetic Properties of Screw Dislocations in Alpha Iron," Energy Frontier Research Centers Forum
- Odbadrakh, Khorgolkhuu (ORNL), Rusanu, Aurelian (ORNL), Stocks, George Malcolm(ORNL), Wang, Yang (Pittsburgh Supercomputing Center), Nicholson, Don M(ORNL), Samolyuk, German D(ORNL), "First Principles Magnetic and Electronic Structure Calculations in Large Non-periodic Dislocation Models," MRS Spring Meeting, 2011.
- Odbadrakh, Khorgolkhuu (ORNL), Nicholson, Don M(ORNL), Rusanu, Aurelian (ORNL), Eisenbach, Markus (ORNL), Evans III, Boyd Mccutchen(ORNL), "First Principles Approach to the Magneto Caloric Effect: Application to Ni₂MnGa," APS March Meeting, 2011.

Publications/Presentations (continued)

- Odbadrakh, Khorgolkhuu (ORNL), Rusanu, Aurelian (ORNL), Stocks, George Malcolm(ORNL), Samolyuk, German D (ORNL), Eisenbach, Markus (ORNL), Wang, Yang (Pittsburgh Supercomputing Center), Nicholson, Don M(ORNL), "Calculated Electronic and Magnetic Structure of Screw Dislocations in Alpha Iron," 55th Annual Conference on Magnetism and Magnetic Materials.
- Pooser, Raphael C(ORNL), Evans, Philip G(ORNL), Earl, Dennis Duncan(ORNL), Williams, Brian P(ORNL), Humble, Travis S(ORNL), "FPGA-based gating and logic for multichannel single photon counting," Single Photon Workshop 2011.
- P.C. Roth and Piotr Luszczek, "Keeneland - Enabling Heterogeneous Computing for the Open Science Community," (2.5 hour presentation) TeraGrid 2011, Salt Lake City, Utah, July 2011.
- P.C. Roth and Piotr Luszczek, "Keeneland - Enabling Heterogeneous Computing for the Open Science Community," (90 minute presentation) Open Grid Forum 32, Salt Lake City, Utah, July 2011.
- Pavel Shamis, Richard L. Graham, Manjunath Gorentla Venkata, Joshua S. Ladd, "Design and Implementation of Broadcast Algorithms for Extreme-Scale Systems," at IEEE Cluster 2011.
- Sullivan, Blair, Using Tree Decomposition for Covariance Selection in Gaussian Graphical Models with Measurement Noise; joint with A. Shojaie*, A. Lenarcic*, M. Mahoney, M. Porter, C. Groer (*presenters) SAMSI opening workshop on Uncertainty Quantification, Raleigh-Durham, NC, September 8, 2011.
- Bobby G. Sumpter "Guiding the Design of Nanostructure Materials," HPC Forum, San Diego, California, Sept. 6-9 (2011).
- Bobby G. Sumpter, "Towards Computational Design of Materials for Energy Science," Materials by Design Workshop, Oak Ridge Sep. 21-22.
- J.S. Vetter, "Emerging Architectures on the Pathway to Exascale Computing," presented at Institute for Nuclear Theory: Extreme Computing and its Applications, Seattle, June 24, 2011.
- J.S. Vetter, "NSF Keeneland Project" presented at NCAR Workshop on Programming weather, climate, and earth-system models on heterogeneous multi-core platforms (Boulder, CO), September 7, 2011.
- Worley, Patrick H(ORNL), "Performance Evaluation and Analysis Consortium (PEAC) End Station," International Conference for High Performance Computing, Networking, Storage and Analysis (SC10).
- Worley, Patrick H(ORNL), Computer Performance of the Community Earth System Model (with A. Craig, J. Dennis, A. Mirin, M. Taylor, and M. Vertenstein), Climate and Earth System Modeling (CESM) Principal Investigator's Meeting, Grand Hyatt Washington Hotel, Washington, DC, September 21, 2011.
- Xing, Yulong (ORNL), "High order accurate DG methods for the generalized Korteweg-de Vries equation," AMS 2011 Spring Western Section Meeting.
- Xing, Yulong (ORNL), "High order numerical methods for the shallow water equations," The International Conference on Applied Mathematics, Modeling and Computational Science.
- Xing, Yulong (ORNL), "Conservative, discontinuous-Galerkin methods for the generalized Korteweg-de Vries equation," The International Conference on Applied Mathematics, Modeling and Computational Science.

Conferences/Workshops

2011 DOE Applied Mathematics Program Meeting

The DOE Office of Advanced Scientific Computing Research (ASCR) will hold a meeting for investigators in the Applied Mathematics Program on October 17-19, 2011 at the Hyatt Regency Reston in Washington, DC. The 2.5-day meeting will consist of a combination of plenary talks, breakout sessions, and poster sessions to highlight recent research in selected theme areas.

The purpose of this meeting is to exchange technical information and foster interactions among researchers funded by the DOE Applied Mathematics Program. Theme areas will be emphasized, but research contributions from all areas of the portfolio of the DOE Applied Mathematics Program are encouraged. The meeting is organized by the Computer Science and Mathematics Division at Oak Ridge National Laboratory.

Theme areas for this meeting include: Linear Algebra, Optimization, Multiscale and numerical PDEs, Discretization and Meshing, Stochastic Systems and Uncertainty Quantification, Analysis of Petascale Data, and Complex Interconnected Systems.

The meeting is funded by the Applied Mathematics Program in the Office of Advanced Scientific Computing Research at DOE.

For more information, please go to <http://www.csm.ornl.gov/workshops/applmath11/>

Fall Creek Falls meeting in Gatlinburg, TN September 13-16

The theme of this year's Fall Creek Falls meeting was "Virtualizing Energy." The first session on Wednesday morning focused on modeling and simulation for energy generation technologies. This session included talks on photovoltaics, small modular reactors, carbon capture and sequestration, grid technologies, and wind. The second session focused on virtualization of the infrastructure, including talks on: transportation, smart grid technologies, batteries, and energy-efficient buildings. After considering the application space in the first two sessions, the focus of the meeting shifted to platforms. The third session considered current and near-term platforms, including talks on the programming model for OLCF3, application preparation for Mira (an IBM/Blue Gene/Q), the Blue Waters programming environment, an update on HPC in China, and an update on the OLCF3 platform. The fourth and final session addressed the software stack for future platforms with an eye toward Exascale platforms. This session included talks on architecture and execution models, file systems and I/O, interoperability of runtime systems, programming models and challenges, and tools to support node level programming.

More information about this meeting, including an agenda with presentations is available at: <http://computing.ornl.gov/workshops/FallCreek11/index.shtml>

Euro-Par 2011 - August 29 - September 2nd

Euro-Par 2011 is organized by National Institute for Research in Computer Science and Control (INRIA), the University of Bordeaux I and the French National Centre for Scientific Research (CNRS). The Euro-Par 2011 conference will be held on the campus of Bordeaux II University, Place de la Victoire, in the center of Bordeaux.

Euro-Par is an annual series of international conferences dedicated to the promotion and advancement of all aspects of parallel and distributed computing.

ORNL was well represented at this year's conference. Stephen Scott served as director of the HPCVirt and Resilience Workshops. Christian Engelmann served as program chair and session chair of the 4th Workshop on Resiliency in High Performance Computing (Resilience) in Clusters, Clouds. Thomas Naughton covered work on virtual machine based fault injection in his presentation "A case for Virtual Machine based Fault Injection in a High-Performance Computing Environment." Siram Lakshminarasimhan and John Jenkins, two students of CSMD researcher and NCSU/ORNL joint faculty member - Nagiza F. Samatova, presented DOE supported papers: "Compressing the Incompressible with ISABELA: In-situ Reduction of Spatio-Temporal Data" and "Lessons Learned from Exploring the Backtracking Paradigm on the GPU" respectively.

For more information about this meeting, please go to <http://europar2011.bordeaux.inria.fr/>

Conferences/Workshops (continued)

NEES/E-Defense Collaborative Earthquake Research Program 9th Planning Meeting

CSMD's John Cobb attended the NEES/E-Defense Collaborative Earthquake Research Program 9th Planning Meeting <<http://peer.berkeley.edu/events/2011/nees-edefense/>> August 26-27, 2011 at the National Research Institute for Earth Science and Disaster Prevention (NIED) E-Defense facility near Kobe, Japan <<http://www.bosai.go.jp/e/>>. This was the latest in a series of ongoing collaborations between large earthquake engineering test facilities and research institutions in the U.S. and Japan, the NIED E-defense facility (supported by the Ministry of Education, Culture, Sports, Science and Technology or MEXT), the George E. Brown Network for Earthquake Engineering Simulation or NEES (funded by the U.S. National Science Foundation, or NSF) <<http://nees.org/>> and the Pacific Earthquake Engineering Research Center or PEER (funded by NSF as well as state and local agencies). <<http://peer.berkeley.edu/>> Sixty-four attendees, primarily from Japan and the U.S., attended the day and a half workshop. There were several excellent technical talks including updated information about the performance of engineered structures during the Great Eastern Japan Earthquake of 2011 and, Cobb, representing the NEES governing board, also attended with Joint Technical Coordinating Committee breakout session for Senior staff where discussions about the future directions of the collaboration were discussed. The highlight of the workshop was its timing to coincide with Prof. Keri Ryan's (University of Nevada Reno) testing on the seismic base isolation and shock absorber damping equipment on a 500-ton, five-story office/hospital structure on the E-Defense table with a ground motion equivalent to the 1995 Kobe earthquake (or Great Hanshin earthquake). The E-Defense shake table is the largest shake table in the world and makes it unique in its ability to investigate seismic response of engineered structures at unprecedented scales.



Five story test building on E-Defense large shake table near Kobe Japan, just before testing of building response to 1995 Kobe-like shaking motions with installed seismic isolation and damping components. This test was conducted during the two day NEES/E-Defense Collaborative Earthquake Research Program 9th Planning Meeting, August 26-27, 2011.

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Group Profile

Application Performance Tools

The Application Performance Tools group conducts research and development and manages vendor interactions in the development and use of software tools and middleware needed to assess and improve application performance on current and emerging HPC systems. The group is primarily focused on issues that arise when using extreme-scale systems and is actively working in the areas of high-performance communication, user- and operating system- level run-time middleware, compiler-based code transformations, file-systems, and performance characterization.

To fully utilize the capabilities of high-end computer systems, we provide the necessary understanding of technical hurdles and the means for surpassing these barriers. We work to ensure an efficient development environment for all aspects of complex scientific application programs.

- Communications Middleware -- Open MPI, Networking research, InfiniBand, collective algorithms, vendor collaborations (Mellanox)
- Compilers based transformations -- Open64, research in compiler feedback/transformations
- Fault tolerance -- Basic R&D in proactive fault tolerance at middleware layers (MPI and below (Colorado State Univ.))
- Benchmarking -- Confidence, important performance measurements with characterize system behavior at scale (latency, noise, etc.)
- Runtime & operating systems -- Basic R&D in highly scalable runtime systems, Scalable Tools Communications Infrastructure (STCI), Colony, GPU aware computing, university collaborations (Univ. of Illinois at Urbana-Champaign)
- Input/Output Middleware -- Removing secondary storage barriers for extreme scale systems, I/O Forwarding Scalability Layer (IOFSL)
- Large-scale debugging -- Allinea Distributed Debugging Tools (DDT), vendor collaborations (Allinea)
- Large-scale tracing -- VampirTrace vendor collaboration (Dresden University of Technology)
- Power/heat aware computing

The Applications Performance Tools group provides both research and support to benefit HPC users with these technologies.



About CSMD

The Computer Science and Mathematics Division (CSMD) is ORNL's premier source of basic and applied research in high-performance computing, applied mathematics, and intelligent systems. Basic and applied research programs are focused on computational sciences, intelligent systems, and information technologies.

Our mission includes working on important national priorities with advanced computing systems, working cooperatively with U.S. industry to enable efficient, cost-competitive design, and working with universities to enhance science education and scientific awareness. Our researchers are finding new ways to solve problems beyond the reach of most computers and are putting powerful software tools into the hands of students, teachers, government researchers, and industrial scientists.

The Division is composed of 10 of Groups. These Groups and their Group Leaders are:

- Computer Science Research - Al Geist
- Future Technologies - Jeff Vetter
- Application Performance Tools - Richard Graham
- Computational Engineering and Energy Sciences - John Turner
- Computational Mathematics - Ed D'Azevedo (Interim)
- Statistics and Data Science - Barney Maccabe (Interim)
- Computational Earth Sciences - Danny McKenna
- Computational Astrophysics - Tony Mezzacappa
- Complex Systems - Jacob Barhen
- Computational Chemical and Materials Sciences - Bobby Sumpter

About this Newsletter

This newsletter is compiled from information submitted by CSMD Group leaders, public announcements and searches.

Please contact Daniel Pack or James Gergel if you have information you would like to contribute.

Contact Information and Links

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LINKS

Computer Science and Mathematics Division - www.csm.ornl.gov

Computing and Computational Sciences Directorate - computing.ornl.gov

Oak Ridge National Laboratory - www.ornl.gov