

2011 CESM Annual Workshop

Almost two dozen researchers from ORNL attended the 16th annual Community Earth Systems Model Annual Workshop. CESM is a fully-coupled, global climate model that provides state-of-the-art computer simulations of the Earth's past, present, and future climate states.

Salishan

The Salishan Conference on HIGH-SPEED COMPUTING was held again in April.

The conference was founded in 1981 as a means of getting experts in computer architecture, languages, and algorithms together to improve communications, develop collaborations, solve problems of mutual interest, and provide effective leadership in the field of high-speed computing.



this issue

Highlights **P.1**

Awards **P.3**

New Faces **P.4**

Publications/Presentations **P.5**

About CSMD **P.6**

Highlights

Gonzalo Alvarez-Campot wins SC early-career research grant



Gonzalo Alvarez-Campot is among three ORNL researchers to receive Office of Science Early-Career Research Program awards. The award is designed to support exceptional researchers during

the crucial early career years, when many scientists do their most formative work. ORNL's grants will be at least \$500,000 per year to cover year-round salary plus research expenses.

Alvarez-Campot, who holds a joint appointments in ORNL's Center for Nanophase Materials Sciences and Computer Science and Mathematics Division (Computational Chemistry and Materials Sciences Group), submitted a winning proposal, titled, "Diagonalization Solvers for Electronic Collective Phenomena in Nanoscience," selected by the Office of Basic Energy Sciences.

This project aims to advance theoretical modeling capabilities to understand nanoscale phenomena in strongly correlated electronic materials, such as high-temperature superconductors. Understanding these materials could provide insights for the development of new materials for solar cells, lighting and power transmission.

Nina Balke, who is also in of the Center for Nanophase Materials Sciences at ORNL, was selected for her proposal, titled, "Spatially Resolved Ionic Diffusion and Electrochemical Reactions in Solids: A Biased View at Lithium-Ion Batteries." While Ezekial A. Unterberg, of ORNL's Fusion Energy Division, submitted "Innovative Techniques for Improved Diagnosis and Control of Edge Localized Modes in 3-D Toroidal Plasmas," selected by the Office of Fusion Energy Sciences.

Packing the ions: Discovery boosts supercapacitor energy storage

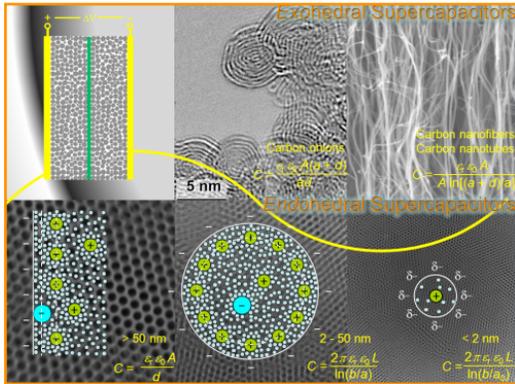
Flat is in the eye of the beholder. When you're talking about nanomaterials, however, that eye is pretty much useless unless it's looking through an electron microscope or at a computer visualization. Yet the pits and ridges on a seemingly flat surface -- so small they are invisible without such tools -- can give the material astonishing abilities. The trick for researchers interested in taking advantage of these abilities lies in understanding and, eventually, predicting how the microscopic topography of a surface can translate into transformative technologies. The team published its findings in the journal *Science*.

"It was a mystery," Sumpter said. "Many people questioned the result at the time. Yet the experimental data was showing an incredible increase in capacitance."

Highlights (continued)

Fortunately, it was a mystery that the ORNL team could unravel.

"We thought this was a perfect case for computational modeling because we could certainly simulate nanometer-sized pores," Sumpter said. "We had electronic-structure capabilities that could treat it well, so it was a very good problem for us to explore."

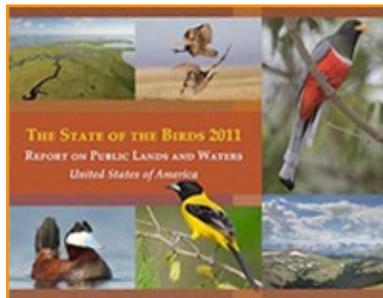


Computational modeling of carbon supercapacitors with the effects of surface curvature included. Credit: Jingsong Huang, ORNL

Using ORNL's Jaguar and Eugene supercomputers, Sumpter and his team were able to take a nanoscale look at the interaction between ion and carbon surface. A computational technique known as density functional theory allowed them to show that the phenomenon observed by Gogotsi was far from impossible. In fact, they found that the ion fairly easily pops out of its solvation shell and fits into the nanoscale pore.

ORNL team aids "State of the Birds 2011" report

Ornithology joined forces with high-performance computing to support a new report on bird habitat released Tuesday by the Secretary of the Interior Ken Salazar and Agriculture Under Secretary Harris Sherman. The "State of the Birds" report relied on lab staff who helped analyze more than 600,000 bird observations collected and logged in Cornell University's eBird database by citizen birders. The report evaluates the distribution of birds on nearly 850 million acres of public land and will be used to set policy agendas for governmental and non-governmental conservation efforts. Through the National Science



Foundation's DataONE (Observation Network for Earth) project, ORNL team members helped integrate volunteer-collected eBird observations with environmental data from land use databases and remote satellite sensing data from the NASA-funded Distributed Active Archive Center at ORNL. With access to NSF's TeraGrid, a collaborative collection of eleven high-performance computing centers, the team was able to calculate bird migration maps with unprecedented detail and accuracy. "Maps of this detail are useful in making land use and other policy decisions that affect habitat for important species," said John Cobb, who leads the ORNL Resource Provider effort for the TeraGrid. While this year's report focused on the relationship between land use and bird habitat, Cobb says future plans include conducting multi-year analyses to better understand how bird migration patterns vary over time, perhaps providing indicators of climate change. ORNL collaborators include Robert Cook and Suresh Santhana Vannan from the Environmental Sciences Division, Bruce Wilson from the Information Technology Services Division, and Line Pouchard and Cobb from the Computer Science and Mathematics Division.

Missile Defense Deputy

Dr. Charles Glover of the Complex Systems Group will be appointed "C2BMC Deputy for Test and Analysis" for the Missile Defense Agency's (MDA) Command, Control, Battle Management and Communications (C2BMC) System. The C2BMC system is a global system that is fielded at present in PACOM (Hawaii), STRATCOM (S. Dakota), NORTHCOM (Colorado), EUCOM (Germany), Israel, Japan, National Capitol Region and Ft. Greely AK. C2BMC receives inputs from all MDA sensors that are distributed around the Earth and in space. It integrates and correlates this information into a common, coherent view of the environment. It then distributes this information to the decision-makers and MDA weapon systems over the global communication network that it built and manages for MDA.

In this position, Dr. Glover is responsible for the development of a strategic test and analysis strategy to field C2BMC's next generation system. This involves aligning the MDA's Integrated Master Test Plan with C2BMC's program development and training plans. Also, he is responsible for overseeing all five phases of each C2BMC test: (1) development of test objectives, (2) test architectures, (3) test and analysis plans, (4) test execution, and (5) test analysis. His team is comprised of about 70 government and industry people.

Awards

Distinguished Employee Program

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

Jingsong Huang (April)

Accomplishment: Jingsong has taken the lead on a project directly targeting advancing the development of multiscale computational tools capable of investigating and optimizing key variables of supercapacitors based on nanoporous carbon materials. The underlying simulations are intimately tied to the computational resources that can only be provided by the enabling capabilities of the NCCS and the carbon materials that comprise the supercapacitors are nanostructured and fit interests at the CNMS. Thus this work bridges three different divisions of ORNL. To date the overall effort has been able to unravel the fundamental role of pore size and shape on the processes relevant to adsorption and energy storage. A quantum mechanical based model that accurately describes the behavior of capacitive energy stored for the entire range of pore sizes (ranging from sub-nanometer to microscopic,) was developed via large-scale calculations [Angew. Chem. Int. Ed. 47(3), 520-524 (2008) and Chem. Eur. J. 112(14), 6614-6626 (2008)]. Remarkably, that model has already been accepted as the state-of-the-art description of carbon based supercapacitors [see Nature Materials 7, 845(2008) and Chemical Society Reviews 38, 2520 - 2531 (2009)]. Additionally the explicit dynamics of the solvation/desolvation processes for the charging and discharging was elegantly examined [ACS Nano. 4(4), 2382-2390 (2010); Micro. Nano. Fluidics 8(5), 703-708 (2010)]. This work is a landmark study that once again demonstrates via large-scale simulation and modeling how electrochemical cell charging in supercapacitors occurs and further develops the 1st theoretic model to take these results into account. The model fully accounts for all of the measured experimental data to-date, including the so-called anomalous capacitance increase for sub-nanometer pores.

Ralf Deiterding (May)

Accomplishment: Development of a new method for simulating ultra-short light pulses in fiber-optical networks. The new method has been verified for a recently published very sophisticated 1000km communication line with heavily dispersion-managed fibers and amplifiers for pico-second pulses. Utilizing the new methods, a first design for the transmission of ultra-fast 100fs pulses and periodic 100fs pulse trains over >100km was demonstrated. The new method has so far been implemented in Mathematica, including evaluation of detailed pulse power and spectrum over distance and time, visualization in 3d plots and animations. Availability of this new method for simulating ultra-fast pulses single-mode communication fiber and its demonstration for unmodulated 1Tb/s communication over more than 100km marks a major milestone for this Durmstrang special program project putting ORNL in position to satisfy all sponsor requirements in designing theoretical prototypes for cutting edge communication lines in minimal time.

Pratul Agarwal (June)

Accomplishment: Received patent for fast computational methods for predicting protein structure from primary amino acid sequence. This 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. The present invention also determines possible intermediates in the protein folding pathway. The present invention has important applications to the design of novel drugs as well as protein engineering. The present invention predicts the three-dimensional structure of a protein independent of size of the protein, overcoming a significant limitation in the prior art.

Recognition

Four researchers from ORNL's Computer Science and Mathematics Division were selected by DOE as winners of the Office of Science's Outstanding Mentor Awards. The winners were: Ralf Deiterding, George Ostrouchov, John Cobb, and Pat Worley

Barney Maccabe served as the General Chair of the 20th International ACM Symposium on High-Performance Parallel and Distributed Computing

Awards (continued)

Fellowships

ODEN FACULTY FELLOW

Cory Hauck (Computational Mathematics) served as a J. Tinsley Oden Faculty Fellow at the Institute for Computational and Engineering Sciences at the University of Texas from April 4-16, 2011. He was invited by Professor Irene Gamba to collaborate on research activities in computational kinetic theory. "

From their website: "[The JTO Faculty Fellow] program's foremost purpose is to bring in outstanding researchers and scholars to the University of Texas to collaborate with ICES faculty, researchers, and students on advanced research in computational engineering, mathematics, and sciences."

New Faces in CSMD



Rahul Sampath

Computational Engineering and Energy Sciences
Computational Scientist

Rahul's specialties are High Performance Parallel Computing, Optimization, and Numerical Analysis



Moetasim Ashfaq

Computational Earth Sciences
Atmospheric Physicist

Moet's research is focused on understanding the nature of interactions among the various components of the climate system.



Seyong Lee

Future Technologies
Computer Scientist

Seyong works in the area of programming systems for heterogeneous architectures.



Srikanth Allu

Computational Engineering and Energy Sciences
Computational Scientist

Primary research involves development of computational techniques for space-time coupled systems based on high order Finite Element formulations and development of numerical strategies for coupled electro-chemical storage systems.



Clayton Webster

Computational Engineering and Energy Sciences
Applied Mathematician and Computational Scientist

His research areas include Applied and Numerical Analysis, Uncertainty Quantification, as well as Verification and Validation.

Publications/Presentations

Publications

- A Parallel Algorithm for the Vehicle Routing Problem, Groër, Chris; Golden, Bruce; Wasil, Edward. *INFORMS Journal on Computing*.
- Long, M.S., W.C. Keene, D.J. Kieber, D.J. Erickson III and H. Maring, "A sea-state based source function for size and composition resolved marine aerosol."
- Cameron-Smith, P.S. Elliott, M. Maltrud, D.J. Erickson III, and O. Wingenter, "Changes in dimethyl sulfide oceanic distribution due to climate change."
- Zepp, R.G., D.J. Erickson III, N.D. Paul and B. Sulzberger, "Effects of solar UV radiation and climate change on biogeochemical cycling: Interactions and feedbacks."
- Kendall, W.J. Wang, M. Allen, T. Peterka, J. Huang, D.J. Erickson III, "Simplified Parallel Domain Traversal," *Proc. of SC'11 (Intl. Conference for High Performance Computing, Networking, Storage and Analysis)*.
- N.S.V. Rao, Y. Narahari, C.E. Veni Madhavan, D.K.Y. Yau, C.Y.T. Ma, An analytical Framework for cyber-physical networks, in *Securing Cyber-Physical Infrastructures: Foundations and Challenges*, Editors: S. Das, K. Kant and N. Zhang.
- Mahajan S., G.R. North, R. Saravanan, M.G. Genton, Statistical Analysis of the Trends in Monthly Heavy Precipitation over the US, *Climate Dynamics*.
- Henry Monti, Ali R. Butt, Sudharshan S. Vazhkudai, "CATCH: A Cloud-based Adaptive Data Transfer Service for HPC," *Proceedings of the 25th IEEE International Parallel & Distributed Processing Symposium*.
- R. Deiterding (CSMD). High-resolution numerical simulation and analysis of Mach reflection structures in detonation waves in low-pressure H₂ - O₂ - Ar mixtures: a summary of results obtained with the adaptive mesh refinement framework AMROC, *Journal of Combustion*.
- E. J. Bochove, A.B. Aceves, Y.Y. Braiman (CSMD), P.R. Colet, R. Deiterding (CSMD), A. Jacobo, C.A. Miller (CSMD), C. Rhodes, S.A. Shakir. Model of the self-Q-switching instability of passively phased fiber laser arrays, *IEEE Journal of Quantum Electronics*.
- Y. Xing and C.-W. Shu, High-order finite volume WENO schemes for the shallow water equations with dry states, *Advances in Water Resources*, to appear.
- Y. Chen, X.-H. Sun, R. Thakur, P.C. Roth, and W.D. Gropp, "LACIO: A New Collective I/O Strategy for Parallel I/O Systems," *2011 IEEE International Parallel and Distributed Processing Symposium*.
- C. McCurdy, J.S. Vetter, P. Worley, and D. Maxwell, "Memphis on a Cray XT: Pinpointing Memory Performance Problems on Cray Platforms," *Proc. Cray Users Group Conference*.
- X. Que, W. Yu, V. Tipparaju, J.S. Vetter, and B. Wang, "Network-Friendly One-Sided Communication Through Multinode Cooperation on Petascale Cray XT5 Systems," *Proc. IEEE International Symposium on Cluster Computing and the Grid*.
- Dong Li, Dimitrios Nikolopoulos, Kirk Cameron, Bronis de Supinski, and Martin Schulz. "Memory Registration for High Performance Networks Using Helper Threads."
- Weikuan Yu, Vinod Tipparaju, Xinyu Que, Jeffrey S. Vetter. "Virtual Topologies for Scalable Resource Management and Contention Attenuation in a Global Address Space Model on the Cray XT5."
- Karol Kowalski, Ryan Olson, Sriram Krishnamoorthy, Vinod Tipparaju, Edoardo Aprà. "The role of many-body effects in describing low-lying excited states of $\frac{1}{4}$ -conjugated chromophores: high-level equation-of-motion coupled-cluster studies of fused porphyrin systems."



Cover Art

Pratul Agarwal's paper "Redox-Promoting Protein Motions in Rubredoxin" on joint neutron scattering and computational study appeared on the cover of *Journal of Physical Chemistry B*, on July 21, 2011.

Publications/Presentations (continued)

- A. A. Mirin and P. H. Worley, "Improving the Performance Scalability of the Community Atmosphere Model," International Journal for High Performance Computer Applications.
- George Bosilca, Aurelien Bouteiller, Anthony Danalis, Thomas Herault, Jack Dongarra, Pierre Lemarinier. "DAGuE: A generic distributed DAG engine for high performance computing." 16th International Workshop on High-Level Parallel Programming Models and Supportive Environments (HIPS).
- George Bosilca, Aurelien Bouteiller, Anthony Danalis, Mathieu Faverge, Azzam Haidar, Thomas Herault, Jakub Kurzak, Julien Langou, Pierre Lemarinier, Hatem Ltaief, Piotr Luszczek, Asim YarKhan, Jack Dongarra. "Flexible Development of Dense Linear Algebra Algorithms on Massively Parallel Architectures with DPLASMA." 12th IEEE International Workshop on Parallel and Distributed Scientific and Engineering Computing.
- Dong Li, Surendra Byna and Srimat Chakradhar. "Energy-Aware Workload Consolidation on GPU." International Workshop on Scheduling and Resource Management for Parallel and Distributed Systems. In conjunction with International Conference on Parallel Processing.
- P. H. Worley, A. P. Craig, J. M. Dennis, A. A. Mirin, M. A. Taylor, and M. Vertenstein, "Performance of the Community Earth System Model," in Proceedings of the ACM/IEEE International Conference for High Performance Computing, Networking, Storage and Analysis.
- X. Wu, K. Vijayakumar, F. Mueller, X. Ma, and P.C. Roth, "Probabilistic Communication and I/O Tracing with Deterministic Replay at Scale," 2011 International Conference on Parallel Processing.
- Weikuan Yu, Vinod Tipparaju, Xinyu Que, and Jeffrey Vetter. Virtual Topologies for Scalable Resource Management and Contention Attenuation in a Global Address Space Model on the Cray XT5. IEEE International Conference on Parallel Processing.
- Karol Kowalski, Sriram Krishnamoorthy, Ryan M. Olson, Vinod Tipparaju, E. Apra, Scalable Implementations of Accurate Excited-state Coupled Cluster Theories: Application of High-level Methods to Porphyrin-based Systems. In Supercomputing, 2011. SC '11. Proceedings of the ACM/IEEE SC 2011 Conference, 2011.
- James Dinan, Sriram Krishnamoorthy, Pavan Balaji, Jeff R. Hammond, Manojkumar Krishnan, Vinod Tipparaju, Abhinav Vishnu. Noncollective Communicator Creation in MPI. IMUDI 2011 Special Session on Improving MPI User and Developer Interaction.
- Andres R. Botello-Mendez, Eduardo Cruz-Silva, Jose M. Romo-Herrera, Florentino Lopez-Urías, Mauricio Terrones, Bobby G. Sumpter, Humberto Terrones, Jean-Christophe Charlier, Vincent Meunier, Quantum Transport in Graphene Nanonetworks, Nano Letters.
- Alejandro Lopez-Bezanilla, Jingsong Huang, Humberto Terrones, Bobby G. Sumpter, Boron Nitride Nanoribbons Become Metallic, Nano Letters.
- 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.
- 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," Physical Chemistry Chemical Physics
- William A. Shelton, Edoardo Aprà, Bobby G. Sumpter, Aldilene Saraiva-Souza, Antonio G. Souza Filho, Jordan Del Nero, Vincent Meunier, Theory of zwitterionic molecular-based organic magnets, Chemical Physics Letters
- Katie Campbell, Bilge Gurun, Bobby G. Sumpter, Yonathan S. Thio, David G. Bucknall, Role of Conformation in π - π Interactions and Polymer/Fullerene Miscibility, J. Phys. Chem. B.
- J. Messman, D. Pickel, D. Uhrig, B. G. Sumpter, M. Goswami, 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.
- E. Cruz-Silva, F. Lopez-Urias, E. Munoz-Sandoval, B.G. Sumpter, H. Terrones, J.C. Charlier, V. Meunier, M. Terrones, M., Phosphorus and phosphorus-nitrogen doped carbon nanotubes for ultrasensitive and selective molecular detection. Nanoscale.

Publications/Presentations (continued)

- M. Goswami, R. Kumar, B. G. Sumpter, J. Mays, Breakdown of Inverse Morphologies in Charged Diblock Copolymers. *Journal of Physical Chemistry B*.
- A. Mladek, J. Sponer, B. G. Sumpter, M. Fuentes-Cabrera, J.E. Sponer, Theoretical modeling on the kinetics of the arsenate-ester hydrolysis: implications to the stability of As-DNA. *Physical Chemistry Chemical Physics*.
- A. Vazquez-Mayagoitia, S.R. Horton, B.G. Sumpter, J. Sponer, J.E. Sponer, M. Fuentes-Cabrera, On the Stabilization of Ribose by Silicate Minerals. *Astrobiology*.
- J.J. Yoo, K. Balkrishnan, J.S. Huang, V. Meunier, B.G. Sumpter, A. Srivastava, M. Conway, A.L.M. Reddy, J. Yu, R. Vajtai, P.M. Ajayan, Ultrathin Planar Graphene Supercapacitors. *Nano Letters*.
- X. Yui, K. Xiao, J.H. Chen, N.V. Lavrik, K.L. Hong, B.G. Sumpter, D.B. Geohegan, High-Performance Field-Effect Transistors Based on Polystyrene-*b*-Poly(3-hexylthiophene) Diblock Copolymers. *Acs Nano*.
- E. Cruz-Silva, Z. M. Barnett, B. G. Sumpter, V. Meunier, Structural, magnetic, and transport properties of substitutionally doped graphene nanoribbons from first principles, *Phys. Rev. B*.
- Y. Zhang, X. Ke, C. Chen, J. Yang, P.R.C. Kent, Nanodopant-induced band modulation in AgPbmSbTe_{2+m}-type thermoelectrics, *Phys. Rev. Lett*.
- Joshua Hursey, Thomas Naughton, Geoffroy Vallee and Richard L. Graham, "A Log-Scaling Fault Tolerant Agreement Algorithm for a Fault Tolerant MPI," at the 18th European MPI Users' Group Meeting, 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.
- 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.
- Mohamad Chaarawi, Edgar Gabriel, Rainer Keller, Richard Graham, George Bosilca and Jack Dongarra. "OMPIO: A Modular Software Architecture for MPI I/O," Accepted to Euro MPI, 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," at the 18th European MPI Users' Group Meeting, 2011.
- Joshua Hursey, Jeffrey M. Squyres and Terry Dontje, "Locality-Aware Parallel Process Mapping for Multi-Core HPC Systems," at IEEE Cluster 2011, 2011.
- C. Y. T. Ma, N. S. V. Rao, 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, D. Rose, Analytical and simulation studies of tactical edge networking on command and control, 9th Annual U. S. Missile Defense Conference, abstract and conference presentation, 2011.
- N. S. V. Rao, J. C. Chin, D. K. Y. Yau, C. Y. T. Ma, Performance trade-offs in distributed detection networks, *INFORMS Computational Science Conference*, abstract and conference presentation, 2011.

Invited Presentations

- Jeffrey S. Vetter. "Emerging Architectures on the Pathway to Exascale Computing," HP-Cast Keynote.
- Jeffrey S. Vetter. "The Under-appreciated Exascale Challenge: Memory and Storage," *International Supercomputing Conference*.
- Jeffrey S. Vetter. "Emerging Architectures on the Pathway to Exascale Computing," *Institute for Nuclear Theory: Extreme Computing and its Applications*.
- Bobby G. Sumpter, "Towards Understanding and Design of Functional Nanostructured Materials," *Chemistry and Dynamics in Complex Environments Workshop*, Telluride June 2011.

Workshop/Session Chair Organization

- Pratul Agarwal and Bobby G. Sumpter, Collaborative Workshop on Bio-catalysis, Denver, CO, May 26 (2011).

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

CONTACTS

CSMD Director -

Barney Maccabe - maccabeab@ornl.gov

Division Secretary -

Lora Wolfe - wolfelm@ornl.gov

Director of Special Programs/Chief Scientist -

Steve Poole - spoole@ornl.gov

ORNL TeraGrid Lead -

John Cobb - cobbjw@ornl.gov

Technical Communications -

Daniel Pack - packdl@ornl.gov

James Gergel - gergelj@ornl.gov

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