

Upcoming Events

The Third Workshop on Data Mining in Earth System Science (DMESS 2012)--co-convened by Forrest M.

Hoffman, Jitendra Kumar, J. Walter Larson, Richard Tran Mills, and Miguel D.

Mahecha--will be held in conjunction with the International Conference on Computational Science (ICCS) on June 4-6, 2012, in Omaha, Nebraska. DMESS 2012 will create a forum for original research papers and presentations from leading computational and earth scientists who are applying data mining techniques on advanced computing platforms (HPC systems, clusters, grids and clouds) to distill knowledge from the massive--and growing--data sets created by the earth science community. The theme for ICCS 2012 is "Empowering Science through Computing," to mark the ever-increasing importance of and progress in computational science theory and practice.



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Highlights

OpenCL Gains Ground On CUDA

A recent article in HPCWire recognizes ORNL's Scalable Heterogeneous Computing benchmarks, which are sponsored by DOE ASCR and NSF, for performance testing on emerging architectures with OpenCL and CUDA. Kyle Spafford from ORNL's Future Technologies group has been benchmarking the two technologies for some time and is now convinced that OpenCL performance is closing the gap on CUDA. He recently presented his findings at Georgia Tech's Keeneland Workshop. Spafford ran ORNL's Scalable Heterogeneous Computing Benchmark Suite (SHOC) that has been optimized for both CUDA and OpenCL, and found that OpenCL can match CUDA performance on most of the basic math kernels. He also found that OpenCL's performance on some kernels, like SGEMM, has increased 10-fold since 2009. The one code that CUDA still has a significant performance advantage is that of the Fast Fourier Transform (FFT). Spafford attributes CUDA's better FFT performance on its use of a fast intrinsic, with AMD's OpenCL employing a slower, more accurate version. If the implementations are matched, the performance difference goes away, says Spafford. [\[Read more here.\]](#)

Next-generation Electronics . . .

Changing the behavior of a material isn't big magic -- it's nanoscale chemistry. Alejandro Lopez-Bezanilla, from CSMD's Computational

Chemical and Materials Sciences Group, used the computing power of Oak Ridge National Laboratory's Jaguar supercomputer, America's fastest, to study the effects of adding oxygen, sulfur and hydrogen to nanoribbons made of boron nitride. The added elements changed the behavior of boron nitride -- a good insulator -- into that of a metal. That makes the material promising for faster computer chips and smarter cell phones. Stable, inexpensive boron nitride can serve as a substrate to support blazing-fast graphene, a material being studied for next-generation electronics. Graphene and boron nitride can be created in 1-atom-thick sheets and cut into ribbons to carry electrons and their on/off electronic messages. [Written by Sandra Allen McLean; media contact: Ron Walli, (865) 576-0226; wallira@ornl.gov]

Researchers Work Recognized

As recognition of the success of their work on climate science problems, CSMD researcher Nagiza Samatova and North Carolina State University (NCSU) professor Fred Semazzi have been chosen by NCSU to appear NCSU's advertisement in Chronicle of Higher Education. Additionally, Drs. Samatova and Alok Choudhary (from Northwestern University) were invited to present their work to the Advanced Scientific Computing Advisory Committee (ASCAC) in March.

Highlights (continued)

Rao Awarded Patent



CSMD researcher and ORNL Corporate Fellow Nageswara Rao was awarded patent number US 8,144,686 B2 for his work

Method and Systems for Bandwidth Scheduling and Path Computation for Connection-Oriented Network. The patent is related to the control server used in a connection-oriented network. The control server receives requests to establish and

utilize dedicated channels in the network. The control server utilizes various scheduling methods and algorithms to determine channels based on the request's requirements and resources of the network. For example, the control server may determine an channel based on:

- a specified bandwidth in a specified time slot,
- highest available bandwidth in a specified time slot,
- earliest available time with a specified bandwidth and duration, and
- all available time slots with a specified bandwidth and duration.

Nanoscale Ferroelectricity in Crystalline γ Glycine

CSMD researchers Nina Balke, Stephen Jesse, Alexander Tselev, Pratul Agarwal, Bobby Sumpter, and Sergei Kalinin were part of a team that used materials synthesis, experiments and computational simulations to produce and investigate the ferroelectric properties of γ glycine. The team was able to show the existence of ferroelectric domains and characterized the ferroelectric switching process for different domains using piezoresponse force microscopy. Density functional theory calculations and force-field based simulations were used to explain the switching process in the glycine molecule, demonstrating molecule rotation and crystallization when electrical fields are applied locally.

Glycine is a material of high significance and interest due to the fact that it is the simplest amino acid and is widely used by living organisms to build proteins. This was the first time ferroelectric properties of γ glycine have been presented. Glycine has been known to be piezoelectric since 1954, but the discovery of reversible polarization change opens new pathways to novel classes of bioelectronic logic and memory devices, where polarization switching is used to record/retrieve information in the form of ferroelectric domains.

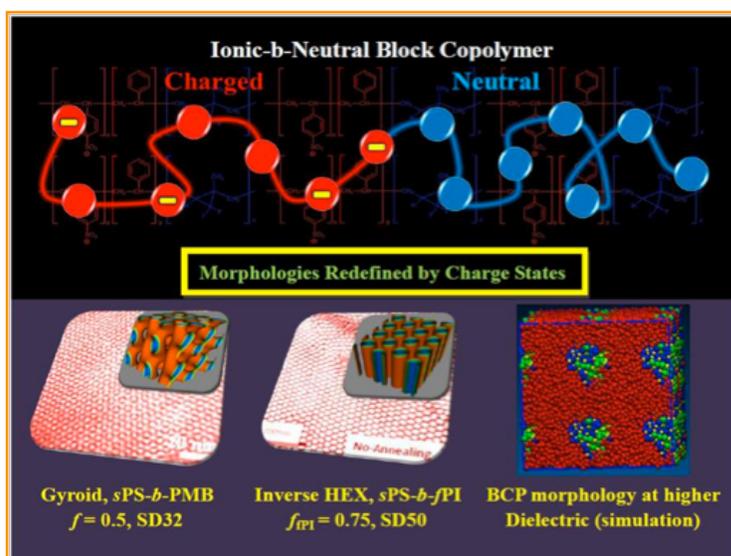
Alejandro Heredia¹, Vincent Meunier², Igor K. Bdikin³, José Gracio³, Nina Balke⁴, Stephen Jesse⁴, Alexander Tselev⁴, Pratul Agarwal⁴, Bobby G. Sumpter⁴, Sergei V. Kalinin⁴, Andrei L. Kholkin¹

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This work was published in *Advanced Functional Materials*. A portion of this Research at Oak Ridge National Laboratory's Center for Nanophase Materials Sciences was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

A New Dimension for Controlling Polymer Morphology (Invited Review)

The use of a new dimension, charge content, to manipulate the morphology of block copolymers is reviewed.¹ Targeted-self-assembly controlled by this new parameter endows block copolymers with even broader technological applications, in areas such as green energy and nanolithography. As is well known, traditionally the nanophase-separated morphology of a block copolymer system is determined by polymer chain length, thermodynamic interactions between components, volume fraction of each component, and macromolecular architecture. Nanophase separation into well-defined



Cover page for forthcoming issue of *Soft Matter* displaying the "abnormal" phase diagram for charged-b-neutral block copolymers: lamellae vs gyroid, hexagonally packed cylinders (HEX) vs inverse HEX. Simulations (right) shows block copolymer morphology at higher dielectric constants.

Highlights (continued)

morphologies has been experimentally well developed and theoretically calculated for neutral polymers. However, incorporation of charges into a block copolymer can dramatically change the rules of phase separation. Charged states and electrostatic interactions significantly affect morphological behavior on a molecular level, which creates a new dimension for manipulating phase behavior as desired. Also, an emerging marriage of ionic liquids or poly(ionic liquids) (ILs, PILs) with block copolymers endows soft matter with broad applications in areas such as catalysis, gas separation media, and energy (e.g. fuel cells and batteries), taking the advantage of the physical scaffold of polymers combined with the ionic nature of ILs/PILs.

This work was supported by Materials Sciences and Engineering Division and the Scientific User Facilities Division (the review includes discussion of work performed as CNMS theme science as well as results from user projects).

Xiaojun Wang, Monojoy Goswami, Rajeev Kumar, Bobby G. Sumpter, Jimmy W. Mays, "Morphologies of Block Copolymers Composed of Charged and Neutral Blocks", invited review for *Soft Matter* 8, 3036 (2012), DOI: 10.1039/c2sm07223h.

Supramolecular Self-Assembly of π -conjugated Hydrocarbons via 2D Cooperative CH/ π Interaction

CSMD researchers Qing Li, Miguel Fuentes-Cabrera, Bobby Sumpter, Petro Maksymovych and Minghu Pan were part of a team that demonstrated a viable pathway toward deterministic control over weak attractive and repulsive interaction between aromatic molecules on a metal surface. There are three key elements in this achievement:

- CH/ π hydrogen bonding among 2D aromatic hydrocarbons on a metal surface is definitively observed for the first time
- Cooperative (multicentric) CH/ π interactions are found to enable supramolecular self-assembly of "magic" chiral molecular clusters with almost perfectly uniform size-distribution
- State-of-the-art first-principle calculations in combination with tunneling spectroscopy are used to reveal emergent electronic properties of supramolecular assemblies

This work is significant as supramolecular self-assembly on well-defined surfaces provides access to a multitude of nanoscale architectures, including clusters of distinct symmetry and size. The driving forces underlying supramolecular structures generally involve both graphoepitaxy and weak directional noncovalent

interactions. In this work, the researchers show that functionalizing a benzene molecule with an ethyne group introduces attractive interactions in a 2D geometry, which would otherwise be dominated by intermolecular repulsion. Furthermore, the attractive interactions enable supramolecular self-assembly, wherein a subtle balance between very weak CH/ π bonding and molecule-surface interactions produces a well-defined "magic" dimension and chirality of supramolecular clusters. The nature of the process is corroborated by extensive scanning tunneling microscopy/spectroscopy (STM/S) measurements and ab initio calculations, which emphasize the cooperative, multi-center character of the CH/ π interaction. This work points out new possibilities for chemical functionalization of π -conjugated hydrocarbon molecules that may allow for the rational design of supramolecular clusters with a desired shape and size.

Qing Li*, Chengbo Han**, Scott R Horton*, Miguel Fuentes-Cabrera*, Bobby G. Sumpter*, Wenchang Lu**, Jerry Bernholc**,†, Petro Maksymovych*, and Minghu Pan*

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†Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee

This work will be published in ACS Nano (DOI: 10.1021/nn203952e). The research was conducted at the Center for Nanophase Materials Sciences (CNMS), which is sponsored at Oak Ridge National Laboratory by the Office of Basic Energy Sciences, U.S. Department of Energy. The work at NCSU was supported by DOE grant DE-FG02-98ER45685. The computations were performed using the resources of the CNMS and the National Center for Computational Sciences at Oak Ridge National Laboratory.

Article to Appear in The Astrophysical Journal

The article "Turbulent Magnetic Field Amplification from Spiral SASI Modes: Implications for Core-Collapse Supernovae and Proto-Neutron Star Magnetization" was accepted for publication in *The Astrophysical Journal* (ApJ) on March 11, 2012.

In this paper, CSMD staff member Eirik Endeve and collaborators used high-resolution MHD simulations to study the role of turbulence induced by the standing accretion shock instability (SASI) in amplifying magnetic fields in the core-collapse supernova environment. They found that the magnetic fields may be efficiently amplified via a SASI-driven turbulent dynamo. They also found that the development of

Highlights (continued)

turbulence may play an important role for the non-linear evolution of the SASI itself. The article is tentatively scheduled for the May 10 issue (arXiv: 1203.3108 [astro-ph.SR]). The findings in the above ApJ paper have initiated a new detailed study of the role of turbulence on the evolution of the SASI. Preliminary results were submitted to Physica Scripta, to the proceedings of the conference "Turbulent Mixing and Beyond 2011" (arXiv: 1203.3748 [astro-ph.SR]).

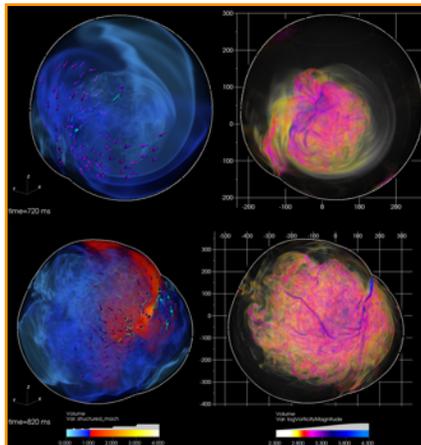


Image sequence illustrating the development of turbulence from the spiral SASI mode in a core-collapse supernova: Mach number (left panels) and vorticity (right panels). The supernova shock surface is traced out by the white contour. Velocity vectors in regions where the flow speed exceeds 10000 km/s are shown in the left panels. (Image created by Ross Toedte, NCCS)

New Faces in CSMD



Manjunath Gorentla Venkata

Application Performance Tools
Software Developer - HPC Tools

Manju's research interests revolve around the design and implementation of system software for massively parallel (MP) systems and clusters, particularly, communication interfaces, protocols, and libraries. Recently, his research focus has been to improve the performance and scalability of collective operations for MP systems, and scalability of Open MPI for Cray XE/XK systems.



Gary Liu

Scientific Data Group
Research Scientist

Gary's major task is to develop fast, portable and scalable I/O solutions that will benefit application codes such as combustion and climate research for DOE leadership computing facilities.

Moving On

Richard Graham

Rich Graham accepted a position with Mellanox. Rich has been with ORNL since January 2007 and was the founding Group leader for the Applications Performance Tools Group in October of 2008. In August 2011, Rich became the Durmstrang Program Director for the Extreme Scale Systems Center.

Chris Groer

Chris Groer was the team lead for the Job Schedulers and Resource Managers effort in the Durmstrang project within the ESSC. Chris and the team wrote a number of reports which compared different schedulers, such as Moab, SLURM and many of the current commercial offerings, on parallel clusters on to evaluate overall performance, energy use and many other vital metrics. Chris worked with Blair Sullivan and a number of team members on developing algorithms to generate tree decomposition of large graphs in support of extreme scale data analysis. Chris now works for the company Link Analytics on the large-scale data analytics of transactions on a variety of data to understand commercial market trends.

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.

January

Norbert Podhorszki worked with Mathieu Gontier from NUMECA International S.A to implement an efficient I/O module for the FineTM/Turbo solver for CFD applications. The new solver has been used by RAMGEN Power Systems, LLC on Jaguar, with a tenfold increase in checkpoint/restart performance, allowing this application to scale much better. The unusual characteristics of the solver is that, for load balancing reasons, each processor holds multiple and a variable number of pieces of each variable because of a non uniform balancing of the structured model over the processes. This renders all traditional I/O solutions very inefficient, especially their original host-slaves IO approach based on CGNS on a very large number of sub domains, and which becomes the bottleneck at scale. The buffering mechanism and the aggregation I/O method provided by ADIOS, combined with an easy-to-use API, helped them to separate the problem of I/O performance from the definition of I/O in the application itself and to provide efficient I/O performance on Jaguar. Additionally, the self-describing data format of ADIOS allows the application to restart from a previous checkpoint on an arbitrary number of processes. In numbers, a computation originally requiring about 2000-sec was optimized until 120-sec with a non negligible memory over consumption, against 40-sec with ADIOS without additional memory.

February

Cory Hauck is the Oak Ridge node leader for Ki-Net, a new research network funded by the NSF for the next five years. Research networks are a new mode of operation under the Division of Mathematical Sciences at the NSF. Their purpose is to facilitate travel and interaction between institutional members. Ki-Net is focused on kinetic theory, primarily on "emerging applications" in quantum dynamics, network dynamics, and biological sciences. It is one of only three funded projects and the only one in applied mathematics.

March

Cindy Sonewald is an exemplary employee that is always willing to help others and strives to deliver the utmost quality and timeliness as a group's administrative assistant. She has built a relationship with all of the groups and no one has a problem with coming to her for help. Cindy has worked above and beyond the call of duty on everything from planning meetings to handling even the most in-depth details of subcontracts so that the researchers can be left to their science. She regularly works overtime to help with proposals, budgets and purchases. And if the programming ever gets the researchers down, they can always go to Cindy for a good laugh or a brief discussion on literary classics for a short break. Cindy's contribution to the group is phenomenal and we wouldn't be the same without here.

Other Awards/Recognition

Clayton Webster Appointed as Editorial Board Member - Twice!



CSDM Researcher Clayton Webster has been appointed as an editor for both the *International Journal for Uncertainty Quantification* (IJUQ) and *SIAM Journal on Uncertainty Quantification* (JUQ).

The *International Journal for Uncertainty Quantification* disseminates information of permanent interest in the areas of analysis, modeling, design and control of complex systems in the presence of uncertainty. The journal seeks to emphasize methods that cross stochastic analysis, statistical modeling and scientific computing. Systems of interest are governed by differential equations possibly with multiscale features. Topics of particular interest include representation of uncertainty, propagation of uncertainty across scales, resolving the curse of dimensionality, long-time integration for stochastic PDEs, data-driven approaches for constructing stochastic models, validation, verification and uncertainty quantification for predictive computational science, and visualization of uncertainty in high-dimensional spaces. Bayesian

computation and machine learning techniques are also of interest for example in the context of stochastic multiscale systems, for model selection/classification, and decision making. Reports addressing the dynamic coupling of modern experiments and modeling approaches towards predictive science are particularly encouraged. Applications of uncertainty quantification in all areas of physical and biological sciences are appropriate.

Awards (continued)

The *SIAM/ASA Journal on Uncertainty Quantification* publishes research articles presenting significant mathematical, statistical, algorithmic, and application advances in uncertainty quantification and related fields such as sensitivity analysis, model validation, model calibration, data assimilation, and code verification. The journal also solicits papers describing new ideas that could lead to significant progress in methodology for uncertainty quantification as well as review articles on particular aspects. The journal is dedicated to nurturing synergistic interactions between the mathematical, statistical, computational, and applications communities involved in uncertainty quantification and related areas

Matt Reuter - 2012 Howes Scholar in Computational Science



Each year one or two recent graduates from the DOE Computational Science Graduate Fellowship program are chosen as the Howes Scholar. This award was established to honor Fredrick Anthony Howes, who managed the Applied Mathematical Science Program in the U.S. Department of Energy during the 1990s. Dr. Howes was highly respected and admired for his energy, dedication and personal integrity.

The awards committee felt that Matt captured the spirit of this award with his “technical excellence, leadership and character.”

There will be a special presentation of the award at the 2012 DOE Computational Science Graduate Fellows conference to be held July 26-28 at the Crystal Gateway Marriott in Arlington, VA.

Conference Report

2012 Ocean Sciences Meeting , Feb. 20-24, Salt Lake City, Utah.

Climate variability of the tropical Atlantic Ocean influences the climate of its surrounding regions by way of Inter Tropical Convergence Zone (ITCZ) variability, the Atlantic Meridional Mode, Atlantic Nino, Benguela Nino, the Atlantic warm pools and tropical cyclogenesis. The tropical Atlantic Ocean itself is influenced by remote forcings such as the El Nino Southern Oscillation (ENSO), Atlantic Meridional Overturning Circulation (AMOC) and the North Atlantic Oscillation (NAO). Recent years have seen a strong improvement in our understanding of tropical Atlantic variability and predictability via paleoclimate and modern observations, high resolution coupled climate modeling and statistical modeling on seasonal to decadal time-scales. However, strong biases still exist in climate models over the tropical Atlantic. The goal of this session was to collectively discuss the current state of knowledge of tropical Atlantic climate variability and identify the research questions critical to a better understanding and prediction of its climate. Abstracts that discussed the variability of the tropical Atlantic, its response to natural and anthropogenic forcings and its influence on the global climate from either a modern or paleo-perspective were encouraged for this session.

The session was co-chaired by Salil Mahajan from the Computational Earth Sciences Group, Computer Science and Mathematics Division and Climate Change Science Institute at Oak Ridge National Laboratory, Takeshi Doi from the Geophysical Fluid Dynamics Laboratory (GFDL), Ernesto Munoz from the National Center for Atmospheric Research (NCAR), and Kelly Kilbourne from the University of Maryland Center for Environmental Science. The session brought together atmospheric scientists and oceanographers from all across the globe to discuss the latest developments in observations and modeling of the Tropical Atlantic. The session included a total of 19 presentations with 7 talks and 11 posters. Prof. R. Saravanan, a leading expert on the tropical Atlantic, from Texas A&M University gave an overview of the current state of understanding and the challenges in modeling and predicting the climate of the region. The presentation in the session ranged from recently derived paleoclimate records to recent observations of the equatorial oceanic currents, analysis of long-term ocean observational data, regional and global climate model biases, and improvements in modeling the region resulting from simulating at high-resolution, and led to several interesting discussions. There were also several presentations and discussions on the coupled atmosphere-ocean free and forced variability - that from modes ENSO, greenhouse gases and aerosols - of the region from the inter-annual to decadal timescales. Overall the session was a success and served as a platform for potential future collaborations to improving our understanding of the climate of the tropical Atlantic and climate predictions.

Community Service

David Bernholdt was a reviewer for the Office of Nuclear Energy Advanced Modeling and Simulation Office SBIR program and the SIAM Journal on Scientific Computing.

Kate Evans attended the Atmospheric Model Working Group meeting to discuss developments in the Community Atmosphere Model component within the CESM. Kate presented recent research as part of the Ultra High Resolution Climate Modeling Project (Jim Hack, PI). [\[More Info.\]](#)

Kate Evans attended the Land Ice Working Group meeting to discuss developments in the Community Ice Sheet Model component within the CESM. Kate presented recent research as part of the Scalable, Efficient, and Accurate CISM (Kate Evans, PI). [\[More Info.\]](#)

Kate Evans gave an invited seminar at Georgia Tech in the Department of Earth and Atmospheric Sciences as part of their seminar series in February.

Kate Evans gave an invited lecture, "Using Computational Science to Understand Earth's Climate," at the NIMBioS STEM lecture/workshop. This workshop is funded by a grant from the National Science Foundation and NIMBioS. This event supports the VolsTeach program. [\[More Info.\]](#)

Al Geist and Kate Evans were members of the organizing committee for the ASCR Extreme Solvers workshop. On March 8-9 in DC. With the committee, Al and Kate planned the agenda and are currently writing a follow-on report about the need for research in the area of solution algorithms for models to effectively utilize ~100PF computers. [\[More Info.\]](#)

Greg Koenig served as a reviewer for the journal *Transactions on Parallel and Distributed Systems*.

Josh Ladd twice guest lectured to Colorado State University's graduate level supercomputing course, "GRAD 511 High Performance Computing & Visualization." Josh also helped professor Pat Burns and his students obtain a class account on Jaguar.

Dong Li served as a program committee member, International Symposium on Cluster Cloud and Grid Computing (CCGrid), 2012

Dong Li served as a program committee member, International Workshop on High Performance, Power-Aware Computing (HPPAC), 2012

Dong Li served as a program committee member, International Conference on P2P, Parallel, Grid, Cloud and Internet Computing (3PGCIC), 2012

Anthony Mezzacappa continued to serve on the Editorial Boards of Computational Science and Discovery and the International Journal of High Performance Computing Applications.

Jeff Vetter worked as the Technical Papers Co-chair for SuperComputing 2012

Jeff Vetter served as a member of papers program committee for InPar 2012

Jeff Vetter served as a member of papers program committee for ICS 2012

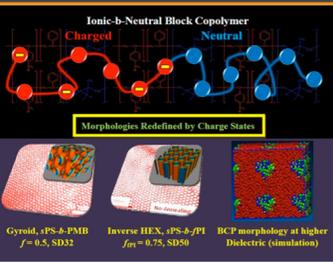
Jeff Vetter served as a member of tutorials program committee for ISC, Tutorials

Clayton Webster and Ed D'Azevedo organized the workshop: ORNL/UTK Numerical Day, March 30. This workshop was co-organized with Xiaobing Feng (UTK) and Yulong Xing. [\[More Info.\]](#)

Publications/Presentations

Papers, Publications, and Presentations

- A. Danalis, C. McCurdy, and J.S. Vetter, "Efficient Quality Threshold Clustering for Parallel Architectures," in *IEEE International Parallel & Distributed Processing Symposium (IPDPS)*. Shanghai: IEEE, 2012.
- A. Danalis, P. Luszczek *et al.*, "BlackjackBench: Portable Hardware Characterization," *SIGMETRICS Performance Evaluation Review*, 40(2), 2012.
- A. Heredia, V. Meunier, I. K. Bdkin, J. Gracio, N. Balke, S. Jesse, A. Tselev, P. Agarwal, B. G. Sumpter, S. V. Kalinin, and A. L. Kholkin, "Nanoscale ferroelectricity in crystalline gamma glycine," *Adv. Func. Mater.*, in press (2012).
- A. Morelos-Gomez, S. Magdalena Vega-Díaz, V. J. González, F. Tristán-López, R. Cruz-Silva, K. Fujisawa, H. Muramatsu, T. Hayashi, X. Mi, Y. Shi, H. Sakamoto, F. Khoerunnisa, K. Kaneko, B. G. Sumpter, YI Ahm Kim, V. Meunier, M. Endo, E. Muñoz-Sandoval, M. Terrones, "Clean Nanotube Unzipping by Abrupt Thermal Expansion of Molecular Nitrogen: Graphene Nanoribbons with Atomically Smooth Edges", *ACS Nano DOI: 10.1021/nn2043252* (2012).
- A. R. Botello-Mendez, E. Cruz-Silva, J. M. Romo-Herrera, F. Lopez-Urias, M. Terrones, B.G. Sumpter, H. Terrones, J.-C. Charlier, V. Meunier "Quantum Transport in Graphene Nanoribbon Networks," APS Meeting Boston, MA Feb. 26-March 2 (2012).
- Alessi, David (Colorado State University, Fort Collins); Wang, Yong (Colorado State University, Fort Collins); Luther, Brad (Colorado State University, Fort Collins); Yin, Liang (Colorado State University, Fort Collins); Martz, Dale (Colorado State University, Fort Collins); Woolston, Mark (Colorado State University, Fort Collins); Liu, Yanwei (University of California, Berkeley & LBNL); Berrill, Mark A (ORNL); Jorge, Rocca (Colorado State University, Fort Collins); "Efficient Excitation of Gain-Saturated Sub-9-nm-Wavelength Tabletop Soft-X-Ray Lasers and Lasing Down to 7.36 nm," *Physical Review X*, 12, 2011, 21023, 1, 2.
- Arthur A. Mirin and Patrick H. Worley, "Improving the performance scalability of the community atmosphere model," *International Journal of High Performance Computing Applications* February 2012 26: 17-30, first published on July 7, 2011 doi: 10.1177/1094342011412630.
- B. G. Sumpter and V. Meunier, "Can Computational Approaches Aid in Untangling the Inherent Complexity of Practical Organic Photovoltaic Systems?," *J. Polymer Sci. B., Polymer Physics*, in press (2012).
- Baker, Christopher G (ORNL); Gallivan, Dr. Kyle A. (Florida State University); Van Dooren, Dr. Paul (Universite Catholique de Louvain); "Low-Rank Incremental Methods for Computing Dominant Singular Subspaces," *Linear Algebra and its Applications*, 4, 2012, 2866, 2888, 436, 8.
- Baker, Christopher G (ORNL); "Supporting Diverse Parallel Models in the Trilinos Library," SIAM Conference on Parallel Processing 2012, Savannah, Georgia.
- Barai, Pallab (ORNL); Nukala, Phani K (ORNL); Sampath, Rahul S (ORNL); Simunovic, Srdjan (ORNL); "Scaling of surface roughness in perfectly plastic disordered media," *Physical Review E*, 2010, 056116-1, 82, 5.



Cover Art

Cover page for forthcoming issue of *Soft Matter* displaying the "abnormal" phase diagram for charged-b-neutral block copolymers: lamellae vs gyroid, hexagonally packed cylinders (HEX) vs inverse HEX. Simulations (above) show block copolymer morphology at higher dielectric constants.

Xiaojun Wang, Monojoy Goswami, Rajeev Kumar, Bobby G. Sumpter, Jimmy W. Mays, "Morphologies of Block Copolymers Composed of Charged and Neutral Blocks", invited review for *Soft Matter* 8, 3036 (2012), DOI: 10.1039/c2sm07223h.

Publications/Presentations

- Bartlett, Roscoe A (ORNL); "TriBITS Lifecycle Model : Version 1.0," 2, 2012
- Berrill, Mark A. (ORNL); Chacon, Luis (ORNL); Philip, Bobby (ORNL). "Adaptive Magnetohydrodynamics Simulations with SAMRAI," 2012, 15th SIAM Conference on Parallel Processing for Scientific Computing, Savannah, Georgia.
- Beste, Ariana (ORNL); Buchanan III, A C (ORNL); "Challenges in the computation of rate constants for lignin model compounds," 1, 2012, 191, 238
- Bisht, Gautam, Forrest M. Hoffman, Jitendra Kumar, Richard T. Mills, and Peter E. Thornton. February 29, 2012. "A Proposed Model Development Strategy to Incorporate 3-D Subsurface Hydrologic and Thermal Processes within the Community Land Model." Community Earth System Model (CESM) Land Model Working Group Meeting (February 29-March 2, 2012), National Center for Atmospheric Research (NCAR), Boulder, Colorado, USA.
- Boboila, Simona (Northeastern University); Kim, Youngjae (ORNL); Vazhkudai, Sudharshan S (ORNL); Desnoyers, Peter (Northeastern University); Shipman, Galen M (ORNL); "Active Flash: Performance-Energy Tradeoffs for Out-of-Core Processing on Non-Volatile Memory Devices," 3, 2012, Proceedings of the 3rd Non-Volatile Memories Workshop, San Diego, California.
- Boehm, Swen (ORNL); Engelmann, Christian (ORNL); "File I/O for MPI Applications in Redundant Execution Scenarios," 2, 2012, 112, 119, 20th Euromicro International Conference on Parallel, Distributed, and network-based Processing (PDP) 2012, Garching.
- C. Han, Q. Li, S. Horton, M. Fuentes-Cabrera, B.G. Sumpter, W.Lu, J. Bernholc, P. Maksymovych, M. Pan, "Computational Study of Supramolecular Self-Assembly Using CH/Pi Bonds," APS Meeting Boston, MA Feb. 27-March 2 (2012).
- Chen, Wei-Chen (ORNL). Maitra, Ranjan (Iowa State University); "Model-Based Clustering of Regression Time Series Data via APECM -- An AECM Algorithm Sung to an Even Faster Beat," Statistical Analysis and Data Mining, 12, 2011, 567, 578, 4, 6.
- Chen, Wei-Chen (ORNL); Ostrouchov, George (ORNL); Pugmire, Dave (ORNL); Prabhat, (Lawrence Berkeley National Laboratory (LBNL)); Wehner, Michael (Lawrence Berkeley National Laboratory (LBNL)); "Applying model-based clustering for analysis of Community Atmospheric Model output," 3, 2012, Conference on Data Analysis (CoDA), Santa Fe, New Mexico.
- Chen, Wei-Chen (ORNL); Ostrouchov, George (ORNL); "High Performance Statistical Computing for Data Intensive Research," 1, 2012.
- Chen, Wei-Chen (ORNL); Ostrouchov, George (ORNL); "pmclust: Parallel Model-Based Clustering," 2, 2012.
- Chen, Yong (Texas Tech University (TTU)); Zhu, Huaiyu (Illinois Institute of Technology); Roth, Philip C (ORNL); Jin, Hui (Illinois Institute of Technology); Sun, Xian-He (Illinois Institute of Technology); "Global-Aware and Multi-Order Context-Based Prefetching for High-Performance Processors," International Journal of High Performance Computing Applications, 11, 2011, 355, 370, 25, 4.
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- X. Wang, M. Goswami, R. Kumar, B. G. Sumpter, J. W. Mays, "Morphologies of Block Copolymers Composed of Charged and Neutral Blocks," invited review for *Soft Matter* 8, 3036 (2012), DOI: 10.1039/c2sm07223h. [Highlight sent and we had the inside cover of the journal]
- Yang Wang (Pittsburgh Supercomputing Center, Carnegie Mellon University); G. Malcolm Stocks (Oak Ridge National Laboratory); Don M. Nicholson (Oak Ridge National Laboratory); Odbadrakh Khorgolkhuu (Oak Ridge National Laboratory); Aurelian Rusanu (Oak Ridge National Laboratory): "Towards ab initio simulation of solid state materials at 10 nm scale," APS March Meeting 2012 Volume 57, Number 1, February 27–March 2 2012; Boston, Massachusetts.
- Yi Zhang (Department of Physics and HiPSEC, University of Nevada, Las Vegas); Xuezhi Ke (Department of Physics, East China Normal University, Shanghai, China); Paul Kent (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory); Changfeng Chen (Department of Physics and HiPSEC, University of Nevada, Las Vegas); Jihui Yang (Materials Science and Engineering Department, University of Washington): "Anomalous Lattice Dynamics in PbTe and Its Implications to Low Intrinsic Lattice Thermal Conductivity," APS March Meeting 2012 Volume 57, Number 1, February 27–March 2 2012; Boston, Massachusetts .
- Yuan Tian, Weikuan Yu, and Jeffrey S. Vetter. "RXIO: Design and implementation of high performance RDMA-capable GridFTP." *Comput Electr Eng* (2011), doi:10.1016/j.compeleceng.2011.11.008.

Invited Presentations

- Deiterding, Ralf (ORNL); "Block-structured adaptive mesh refinement - theory, implementation and application," ESAIM Proceedings, 12, 2011, 97, 150, 34, Summer school on multiresolution and adaptive mesh refinement methods, Frejus.
- Dennis, John (National Center for Atmospheric Research (NCAR)); Edwards, Jim (IBM and National Center for Atmospheric Research); Evans, Kate J. (ORNL); Guba, O. (Sandia National Laboratories (SNL)); Lauritzen, Peter (National Center for Atmospheric Research (NCAR)); Mirin, Art (Lawrence Livermore National Laboratory (LLNL)); St.-Cyr, Amik (National Center for Atmospheric Research (NCAR)); Taylor, Mark (Sandia National Laboratories (SNL)); Worley, Patrick H (ORNL); "CAM-SE: A scalable spectral element dynamical core for the Community Atmosphere Model." *International Journal of High Performance Computing Applications*, 2, 2012, 74, 89, 26, 1 Mountain, GA March 29-30 (2012).
- Guy, Robert (University of California, Davis); Philip, Bobby (ORNL); "A multigrid method for a model of the implicit immersed boundary equations," *Communications in Computational Physics*, 2, 2012, 378, 400, 12, 2.

Publications/Presentations (continued)

- Kumar, Rajeev (ORNL); Goswami, Monojoy (ORNL); Mays, Jimmy (ORNL); Sumpter, Bobby G (ORNL); Wang, Xiaojun (ORNL); "Morphologies of block copolymers composed of charged and neutral blocks," *Soft Matter*, 3, 2012, 3036, 8.
- Li, Dong (ORNL); Cameron, Kirk W. (Virginia Polytechnic Institute and State University (Virginia Tech)); Nikolopoulos, Dimitrios (FORTH-ICS); de Supinski, Bronis R. (Lawrence Livermore National Laboratory (LLNL)); Schulz, Martin (Lawrence Livermore National Laboratory (LLNL)); "Scalable Memory Registration for High-Performance Networks Using Helper Threads," 2011, In Proceedings of ACM International Conference on Computer Frontier (CF).
- Lott, P Aaron (Lawrence Livermore National Laboratory (LLNL)); Elman, Howard (University of Maryland); Evans, Kate J (ORNL); Li, X S (Lawrence Berkeley National Laboratory (LBNL)); Salinger, Andy (Sandia National Laboratories (SNL)); Woodward, Carol (Lawrence Livermore National Laboratory (LLNL)); "Recent Progress in Nonlinear and Linear Solvers," 7, 2011, SciDAC 2011, Denver, Colorado.
- Pouchard, Line Catherine (ORNL); Palanisamy, Giri (ORNL); Cook, Robert B (ORNL); Green, Jim (Information International Associates); Noy, Natasha (Stanford University); "Semantic technologies improving the recall and precision of the Mercury search interface," 2, 2012.
- Pouchard, Line Catherine (ORNL); "Linking Earth and Climate Science for Data Discovery," Spring 2012 Semantic Technology Symposium Series, Charleston, South Carolina.
- Sumpter, Bobby "Guiding the Design of Graphitic Materials for Efficient Energy Storage and Conversion," American Carbon Society Workshop, Stone
- Webster, Clayton - Colloquium: Department of Mathematics: McMaster University - March 7, 2012.
- Webster, Clayton - Colloquium: Department of Mathematics: Tulane University - January 19, 2012.
- Webster, Clayton - Invited Panel: SOS16: "Quantifying the cost of exascale," March 15, 2012.
- Webster, Clayton - Invited talk: "Scientific Computing around Louisiana," (SCALA) - January 21, 2012.

News

David Bernholdt Interim Group Leader for APT

Prior to taking over the Application Performance Tools Group, David spent more than 11 years at ORNL in the Computer Science Research Group. Before that he spent five years as a researcher in the Northeast Parallel Architectures Center at Syracuse University, and nearly three years as a postdoctoral fellow at the Pacific Northwest National Laboratory.

David's research interests center on a broad spectrum of computer science issues that have direct contact with large-scale computational science and engineering applications. This includes software architecture and engineering; parallel programming models, languages, and transformation tools; and fault tolerance, among others.

Having received his formal training and spent the initial part of his research career as a computational chemist, David understands well the perspective of the computational scientists he works with, and the practical challenges they face. He enjoys working in multidisciplinary teams focused on the development of cutting-edge scientific applications which raise many interesting computer science research opportunities.

David currently leads a project on source-to-source code transformation tools for the ASCR exascale research program. He also leads Capability Transfer for the Nuclear Energy Advanced Modeling and Simulation program within the Office of Nuclear Energy. He has led the computer science component of a SciDAC team working on coupled multiphysics simulation of fusion plasmas, and plays a similar role in two pending fusion proposals. David also leveraged this application connection to provide a testbed to demonstrate fault awareness and fault tolerance capabilities for an ASCR project on resilience. Other recent work includes studying the expressiveness of new parallel programming languages for scientific applications, which has had several sponsors, and the development of sophisticated domain-specific languages for a class of problems in quantum chemistry.

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Group Profile

Scientific Data Group

Our mission is to develop cutting-edge statistical and information technologies and to bring quantitative rigor and efficiency to scientific investigations.

We conduct research in the analysis and exploration of data, the collection and organization of data, and decisions based on data. Our collaborative work concerns all stages of the scientific life cycle and utilizes computing platforms ranging from the desktop to large clusters and supercomputers. We team on projects ranging from small single discipline efforts to large multi-disciplinary and multi-institution partnerships.

Areas of application have included:

Chemistry, Biology and Genomics, Astrophysics, Climate, Environmental Science, National Security, Forensics, Simulation Science, Epidemiology, Fusion Science, Transportation and Automotive, Health and Safety, Grid Technologies, Manufacturing, Future Combat Systems, Remote Sensing, Computer Network Security



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 - David Bernholdt (Interim)
- Computational Engineering and Energy Sciences - John Turner
- Computational Mathematics - Ed D'Azevedo (Interim)
- Statistics and Data Science - Scott Klasky
- 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 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