ISSUE
05
SUMMER
2012

QUARTERLY NEWSLETTER FOR THE COMPUTER SCIENCE AND MATHEMATICS DIVISION

CSMD

WWW.CSM.ORNL.GOV

this issue

Highlights P.1
New Faces P.4
Moving On P.4
Awards P.5
Community Service P.6
Publications/Presentations P.8
About CSMD P.16

Upcoming Events

2012 IEEE High Performance Extreme Computing Conference (HPEC '12)
10 - 12 September 2012
Waltham, MA USA

The conference covers advances in high performance extreme computing technologies, emphasizing the following topics:

- Advanced Multicore Software Technologies
- Automated Design Tools
- Mapping and Scheduling of Parallel and Real-Time Applications
- Case Studies and Benchmarking of Applications
- Computing Technologies for Challenging Form Factors
- ASIC and FPGA Advances
- Open System Architectures
- Networking Interconnects and Distributed Computing
- Fault-Tolerant Computing
- Embedded Cloud Computing
- Digital Front Ends
- General Purpose GPU Computing
- Advanced Processor Architectures
- Data Intensive Computing
- New Application Frontiers
- Anti-Tamper Technologies

Highlights

Covalently bonded three-dimensional carbon nanotube solids via boron induced nanojunctions

Achievement

This work exemplifies collaborative nanoscience research between multiple institutions to pioneer the bulk synthesis of 3D macroscale nanotube elastic solids directly via a boron-doping strategy in chemical vapor deposition, that influences the formation of atomic-scale ''elbow'' junctions and nanotube covalent interconnections. The enabling aspect of boron doping was elucidated from detailed theoretical calculations and validated by elemental analysis, revealing that boron promotes formation of negative curvature "elbow'' junctions that leads to robust interwoven 3D networks, a "sponge-like" monolith. This novel material possesses ultra-light weight, super-hydrophobicity, high porosity, thermal stability, and mechanical flexibility, and is strongly oleophilic. These properties enable it as a reusable sorbent scaffold for efficiently removing oil from contaminated seawater.

Significance

The efficient, inexpensive and facile method developed is capable of producing bulk quantities of 3D carbon materials that have broad implications for practical material applications such as selective sorbent materials, hydrogen storage and flexible

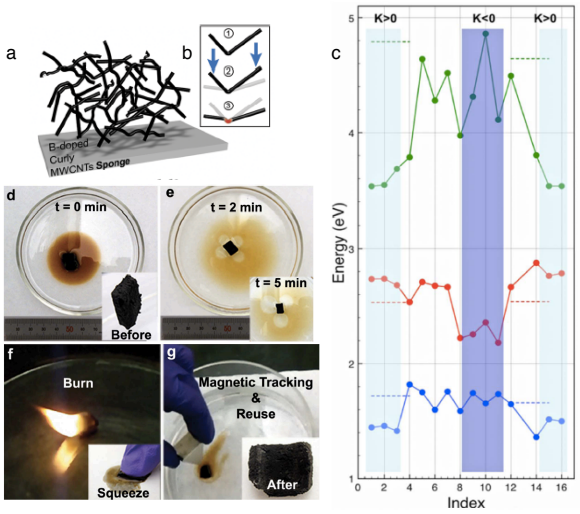


Figure: a,b *A model showing the entangled sponge network;* ***c*** *Relative substitutional energies computed for B, N, and S dopants are shown at different curvatures on a nanotube;* ***d*** *sponge dropped into the oil at t=0, inset shows sponge before use;* ***e*** *sponge sample absorbing the oil at t = 2 min, inset shows t=5 min;* ***f*** *burning or squeezing (inset) out the oil;* ***g*** *reused repetitively and a magnet can track or move the oil.*

conductive scaffolds as porous 3D electrodes. The ultra-lightweight solid material exhibits enabling multifunctional properties including robust elastic mechanical properties with high damping, electrical conductivity, thermal stability, high porosity, super-hydrophobicity, oleophilic behavior and strong ferromagnetism. The environmental oil removal-and-salvage application from seawater was demonstrated where the

OAK RIDGE National Laboratory

nanotube "sponge" acts as an efficient scaffold that can be controlled and recollected via a magnetically driven process, and reused multiple times.
Credit – This work was published in Nature Sci. Rep. 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.
"Covalently bonded three-dimensional carbon nanotube solids via boron induced nanojunctions", D.P. Hashim, N.T. Narayanan, J.M. Romo-Herrera, D.A. Cullen, M.G. Hahm, Peter Lezzi, Joseph R. Suttle, Doug Kelkhoff, E. Munoz-Sandoval,S. Ganguli, A.K. Roy, D.J. Smith, R. Vajtai, B.G. Sumpter, V. Meunier, H. Terrones, M. Terrones, P.M. Ajayan, Nature Sci, Rep. (2012).

ORNL ADIOS team releases version 1.3 of Adaptive Input/Output System

What good are supercomputers if you have to spend your whole time getting data in and out? Researchers at Oak Ridge National Laboratory (ORNL) are working to say goodbye to input/output (I/O) problems with their most recent upgrade of the Adaptive Input/Output System (ADIOS).

ADIOS grew out of a 2008 collaboration between the Oak Ridge Leadership Computing Facility (OLCF) and researchers from academia, industry, and national laboratories. Their goal was a system to get information in and out of a supercomputer efficiently.

"The measurement of success for us has always been 'what percentage of time do you spend in I/O?'" said OLCF computational scientist Scott Klasky. ADIOS was inspired by Klasky's work at the Princeton Plasma Physics Laboratory, where he noticed up to 30 percent of researchers' computational time was spent reading and writing analysis files.

The open-source middleware is designed to help researchers maximize their allocations on leadership-class computing resources from wherever they may be. In essence, it creates more time for research by minimizing the time needed to read and write data to files, even if researchers are sending those files from thousands of miles away.

The previous release—version 1.2—improved usability by allowing users to construct new variables in their simulations while they run, simplifying the interface users work with and improving I/O performance. In fact, researchers using the middleware found the writing process substantially expedited, consuming only .06 percent of their computation time on average.

The biggest challenge for the newest release—version 1.3—was to improve reading efficiency, according to Qing Liu, a scientific researcher working in the Remote Data Analysis and Visualization branch at the National Institute for Computational Sciences and the leading developer of ADIOS. "Our users were very happy that the writing was greatly improved [with version 1.2]. They could get 30 gigabytes per second for the writing performance, but when they tried to read, the performance was much lower," he said. "There was a huge gap between writing and reading performance."
Ray Grout, a researcher at the National Renewable Energy Laboratory, was one of the first people to test the latest update, using the S3D combustion code to study turbulent flows reacting to one another. Grout noted a huge increase in reading performance.

Klasky also added that ADIOS 1.4 will continue grass-root collaboration from computer science researchers to greatly reduce the problem of coping with large data on high-performance machines.

In addition to Klasky, Liu, and Grout, ADIOS 1.3 collaborators include William Tang, C.S. Chang, Weixing Wang, Stephane Ethier, and Zhihong Lin of the Princeton Plasma Physics Laboratory; Norbert Podhorszki, Jeremy Logan, Sean Ahern, Luis Chacon, Roselyne Tchoua, and Ricky Kendall of ORNL; Jackie Chen, Kenneth Moreland, Jay Lofstead, Ron Oldfield, and Todd Kordenbrock of Sandia National Laboratories; Xiaosong Ma, Nagiza Samatova, and Sriram Lakshminarasimhan of North Carolina State University; Garth Gibson and Milo Polte of Carnegie Mellon University; Karsten Schwan and Greg Eisenhauer of Georgia Tech; Hasan Abbasi of the University of Tennessee–Knoxville; Seung-Hoe Ku of New York University; John Wu, Arie Shoshani, and Jinoh Kim of Lawrence Berkeley National Laboratory; Weikuan Yu and Yuan Tian of Auburn University; Manish Parashar, Ciprian Docan, and Fan Zhang of Rutgers University; and Julian Cummings of the California Institute of Technology.
Source: http://www.hpcwire.com/hpcwire/2011-07-21/ornl_adios_team_releases_version_1.3_of_adaptive_input_output_system.html

Highlights (continued)

Package allows analysis and visualization on the fly via Web

Computational scientists have a new weapon at their disposal. Earlier this year, the Electronic Simulation Monitoring (eSiMon) Dashboard version 1.0 was released to the public, allowing scientists to monitor and analyze their simulations in real-time. Developed by the Scientific Computing and Imaging Institute at the University of Utah, North Carolina State University, and Oak Ridge National Laboratory (ORNL), this "window" into running simulations shows results almost as they occur, displaying data just a minute or two behind the simulations themselves. Ultimately, the Dashboard allows the scientists to worry about the "science" being simulated, rather than learn the intricacies of high-performance computing such as file systems and directories, an increasingly complex area as leadership systems continue to break the petaflop barrier.
"In my experience, Dashboard has been an essential tool for monitoring and controlling the large-scale simulation data from supercomputers," said Seung-Hoe Ku, an assistant research professor at New York University's Courant Institute of Mathematical Sciences who uses the Dashboard to monitor simulations of hot, ionized gas at the edge of nuclear fusion reactors, an area of great uncertainty in a device that could one day furnish the world with a nearly limitless abundance of clean energy. "The FLASH interface provides easy accessibility with Web browsers, and the design provides a simple and useful user experience. I have saved a lot of time for monitoring the simulation and managing the data using the Dashboard together with the EFFIS framework."

According to team member Roselyne Tchoua of the Oak Ridge Leadership Computing Facility (OLCF), the package offers three major benefits for computational scientists: first and foremost, it allows monitoring of the simulation via the Web. It is the only single tool available that provides access and insight into the status of a simulation from any computer on any browser; second, it hides the low-level technical details from the users, allowing the users to ponder variables and analysis instead of computational elements; and finally, it allows collaboration between simulation scientists from different areas and degrees of expertise. In other words, researchers separated geographically can see the same data simultaneously and collaborate on the spot.

Furthermore, via easy clicking and dragging, researchers can generate and retrieve publication-quality images and video. Hiding the complexity of the system creates a lighter and more accessible Web portal and a more inclusive and diverse user base.

The interface offers some basic features such as visualizing simulation-based images, videos and textual information. By simply dragging and dropping variable names from a tree view on the monitoring page onto the main canvas, users can view graphics associated with these variables at a particular time stamp. Furthermore, they can use playback features to observe the variables changing over time.
Researchers can also take electronic notes on the simulation as well as annotate movies. Other features include vector graphics with zoom/pan capabilities, data lineage viewing, and downloading processed and raw data onto local machines. Future versions will include hooks into external software and user-customized analysis and visualization tools.
"We are currently working on integrating the eSiMon application programming interface into an ADIOS method so that ADIOS users automatically get the benefit of monitoring their running simulation," said the OLCF's Scott Klasky, a leading developer of ADIOS, an open-source I/O performance library.

The "live" version of the dashboard is physically located at Oak Ridge National Laboratory (ORNL) and can be accessed with an OLCF account at https://esimmon.ccs.ornl.gov. This version of the dashboard gives an overview of ORNL and National Energy Research Scientific Computing Center computers. Users can quickly determine which systems are up or down, which are busy and where they would like to launch a job. Users can also view the status of their running and past jobs as well as those of their collaborators.

However, a portable version of eSiMon is also available for any interested party, and the platform cuts across scientific boundaries so that the Dashboard can be used for any type of scientific simulation. For information on acquiring and/or using the eSiMon dashboard, visit http://www.olcf.ornl.gov/center-projects/esimmon/.
Source: http://www.hpcwire.com/hpcwire/2011-02-28/olcf_partners_release_esimon_dashboard_simulation_tool.html

New Faces in CSMD

Michael Brim

Application Performance Tools
Software Developer - HPC Tools

Michael joined the Application Performance Tools group in May as an HPC Tools Developer. He recently completed his Ph.D. in Computer Sciences at the University of Wisconsin-Madison, where he investigated methods for improving the scalability of tools and middleware for extreme-scale computing environments. His research interests include scalable communication infrastructures and runtime environments, distributed and parallel file systems, and tools for performance analysis and debugging of parallel applications.

Sarah Powers

Application Performance Tools
Research Scientist

Sarah joined ORNL as a Research Scientist in the Application Performance Tools group. She is currently working on scheduling algorithms for HPC applications. Her research interests span a variety of areas related to operations research and applied mathematics such as modeling & simulation, optimization, algorithms, including their scalability as well as speedup and visualization techniques for 'big data' problems.

Moving On

Sylvain Nintcheu Fata

Sylvain Nintcheu Fata was a research staff in the Computational Mathematics Group working on the development of Galerkin boundary integral methods (BIM) and fast pre-corrected FFT boundary element methods (BEM). BEM requires discretization only on the domain surface and is used for modeling problems with moving boundaries such as droplet formation or following crack propagation in materials. Sylvain is the main developer of the boundary element software for solving elliptic partial differential equations at the Integral Equation Technology web site (www.intetec.org). Sylvain is currently exploring opportunities in industry and academic positions.

Olaf Storaasli

Olaf Storaasli retired from ORNL in May 2012. Olaf joined ORNL in 2005 to work on emerging architectures after a distinguished career at NASA Langley. Olaf will continue to live in Oak Ridge.

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.

May

Forrest Hoffman - When the Climate SciDAC call was announced it became obvious that instead of the large monolithic proposals that had been funded in previous calls, DOE was looking for smaller more focused proposals. This opened the door for competition from new players interested in winning support but also threatened to undermine the longstanding cooperation between ORNL and some of the other principal Labs in Climate. Thus, the landscape for negotiating the collaboration between many of the partners became much more complex and uncertain. Forrest was asked to serve as the ORNL point of contact for the definition phase which involved several meetings to negotiate the content of several SciDAC themes mostly in content areas where Forrest had no personal interest and no prospect of support for himself. When the negotiations were complete Forrest had managed to help define three subject areas in biogeochemistry, multiscale processes and ice sheets. Forrest and others at ORNL were then able to bid for and win support for work in all three defined SciDAC Climate areas. Furthermore, Forrest was able maintain the positive and collaborative atmosphere between ORNL and the other labs principally involved in climate science. This epitomizes the selfless leadership we sometimes ask of our staff; Forrest had to look to the bigger picture and not just focus narrowly on his own research interests and needs.

June

Qing Gary Liu, has been performing research in High-performance I/O and has been developing the ADaptable I/O System (ADIOS) software. ADIOS is going to reach its 5th release since 2008 and Gary has continuously improved it. His aggregation strategy to write data out has proved to be the fastest technique at scale at OLCF, therefore all applications that turned to use ADIOS due to their I/O problems, ended up exclusively using his method for running on 100k cores and up. S3D, a combustion simulation code from Sandia has been using ADIOS since before the first release, and has been a driving application for ADIOS. Gary has been the main contact for I/O related work with the authors at Sandia and has been improving their I/O. Gary is an extremely dedicated asset to the Scientific Data Group, who makes sure that ADIOS is high-quality software and is always ready to help applications pushing the limits of I/O on our petascale systems.

In the last month Gary worked nonstop to lead the ADIOS effort to get our next major release, which included I/O staging and new and enhanced reading. He has also worked to assist the S3D team, lead by Jackie Chen, to have high performance I/O.

Other Awards/Recognition

Student Wins ACM Student Research Competition!

Auburn University student Yuan Tian won first place in the graduate category at the Association for Computing Machinery's (ACM) student research competition for her paper "Smart-IO: System-Aware Two-Level Data Organization for Efficient Scientific Analytics." Yuan is currently working in CSM's Scientific Data Group which is led by Dr. Scott Klasky. Dr. Klasky was pleased to point out that Yuan "has been integral for our continued success with ADIOS, and I believe she will be an incredible success in the future, as a postdoctoral scholar in the NSF RDAV project."

Community Service

Brad Settlemyer, reviewer for the Network Research Program of the DOE Office of Advanced Scientific Computing Research

Christian Cardall served as an organizer for the Core-Collapse Supernovae: Models and Observable Signals program at the Institute for Nuclear Theory

Christian Engelmann, program committee [and program chair] for 5th Workshop on Resiliency in High Performance Computing (Resilience) in Clusters, Clouds, and Grids at the 18th International European Conference on Parallel and Distributed Computing (Euro-Par) 2012

Christian Engelmann, program committee, 12th International Conference on Algorithms and Architectures for Parallel Processing (ICA3PP) 2012

Christian Engelmann, program committee, 14th IEEE International Conference on High Performance Computing and Communications (HPCC) 2012

Christian Engelmann, program committee, 2nd International Workshop on Runtime and Operating Systems for Supercomputers (ROSS) 2012, in conjunction with the ACM International Conference on Supercomputing (ICS) 2012

Christian Engelmann, program committee, 7th International Conference on Availability, Reliability and Security (ARES) 2012

Christian Engelmann, reviewer, IEEE Transactions of Parallel and Distributed Systems (TPDS)

Christian Engelmann, reviewer, Journal of Computational Science (JOCS)

Christian Engelmann, reviewer, Journal of Parallel and Distributed Computing (JPDC)

Christian Engelmann, reviewer, Journal of Parallel Computing (PARCO)

Dong Li, committee member for the poster session of the International Conference on Parallel Processing (ICPP), 2012

Dong Li, program committee member for Euro'MPI, 2012

Dong Li, program committee member for the International Workshop on Power Grid-Friendly Computing, 2012

Geoffroy Vallee, program committee for 5th Workshop on Resiliency in High Performance Computing (Resilience) in Clusters, Clouds, and Grids at the 18th International European Conference on Parallel and Distributed Computing (Euro-Par) 2012

Jeffrey S. Vetter is the SC12 Co-Chair for Technical Papers

Jeremy Meredith, program committee member for Symposium on Application Accelerators in High-Performance Computing (SAAHPC) 2012

Patrick Worley was co-organizer and co-chair of the Software Engineering Working Group meetings at the 7th Annual Community Earth System Model Workshop, Breckenridge, CO June 18-21, 2012

Patrick Worley, member of onsite review panel for 2012 DOE Office of Science Graduate Fellowship Program, attended onsite review April 19-20.

Patrick Worley, member of program committee for SC12, attended SC12 program committee meeting on June 24-26

Philip C. Roth, program committee member, 10th IEEE International Symposium on Parallel and Distributed Processing with Applications (ISPA 2012)

Philip C. Roth, program committee member, 17th International Workshop on High-Level Parallel Programming Models and Supportive Environments (HIPS 2012)

Philip C. Roth, program committee member, 28th IEEE Conference on Massive Data Storage (MSST 2012)

Community Service (continued)

Philip C. Roth, program committee member, Second International Workshop on High-Performance Infrastructure for Scalable Tools (WHIST 2012)

Philip C. Roth, program committee member, Third International Workshop on Parallel Software Tools and Tool Infrastructures (PSTI 2012)

Philip C. Roth, reviewer, International Conference on Parallel Architectures and Compilation Techniques (PACT) 2012

Seyong Lee, external reviewer for the International Conference on Parallel Architectures and Compilation Techniques (PACT), 2012

Stephen Scott, program committee [and general co-chair] for 5th Workshop on Resiliency in High Performance Computing (Resilience) in Clusters, Clouds, and Grids at the 18th International European Conference on Parallel and Distributed Computing (Euro-Par) 2012

Sudharshan Vazhkudai, program committee for 5th Workshop on Resiliency in High Performance Computing (Resilience) in Clusters, Clouds, and Grids at the 18th International European Conference on Parallel and Distributed Computing (Euro-Par) 2012

Sudharshan Vazhkudai, program committee, Cluster 2012

Terry Jones, program committee for Improving MPI User And Developer Interaction (IMUDI), 2012

Thomas Naughton, program committee for 5th Workshop on Resiliency in High Performance Computing (Resilience) in Clusters, Clouds, and Grids at the 18th International European Conference on Parallel and Distributed Computing (Euro-Par) 2012

Tony Mezzacappa served on the Editorial Board for Computational Science & Discovery joural

Tony Mezzacappa served on the Editorial Board for International Journal of High Performance Computing Applications

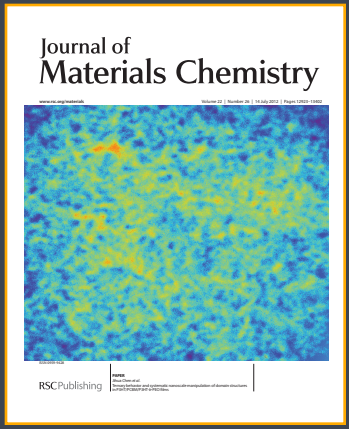
Wael Elwasif, reviewer for the Basic Science Support Project program of the Chalmers e-Science Center at Chalmers University (Sweden)

News

Shipman Joins CSMD

Galen Shipman has joined the Computer Science and Mathematics Division as the Data System Architect for CCSD. His primary responsibility is to develop a system architecture that will support the current and future data requirements of the ORNL S&T mission. His first task is the completion of an ORNL data strategy which he has been developing with Al Geist, based on a set of meetings that were held earlier this year. Needless to say, Galen will be working closely with several of the Groups in the CSMD to ensure that the resulting infrastructure will support our research efforts.

Galen will also work with several of the Groups in NScD, NCCS, CSED and the ITSD on data intensive projects. Prior to coming to the CSMD, Galen served as the leader of the Technology Integration Group in NCCS and thought briefly about taking an industrial position. In the past year, Galen has been directly involved in addressing the data infrastructure needs for the NCCS, SNS and for the Climate modeling community.



Cover Art

Cover page for forthcoming issue of *Journal of Materials Chemistry* displaying an energy filtered TEM image of ternary behavior and systematic nanoscale manipulation of domain structures in P3HT/PCBM/P3HT-b-PEO films.

Jihua Chen , Xiang Yu , Kunlun Hong , Jamie M. Messman , Deanna L. Pickel , Kai Xiao , Mark D. Dadmun , Jimmy W. Mays , Adam J. Rondinone , Bobby G. Sumpter and S. Michael Kilbey II J. Mater. Chem., 2012,22, 13013-13022 DOI: 10.1039/C2JM31124K

Publications/Presentations

Conference Abstracts

- Archibald, Richard K. (ORNL); "Uncertainty Quantification Methods for High Performance Computing: Scalable Approximation and Error Estimation for Stochastic Collocation" 5/2012, SAMSI Transition Workshop, Research Triangle Park, North Carolina
- Archibald, Richard K. (ORNL), Chakoumakos, Madison (ORNL), Zhuang, Zibo (ORNL); "Characterizing the elements of Earth's radiative budget: Applying uncertainty quantification to the CESM" 2012, ICCS 12, Omaha, Nebraska
- Archibald, Richard K. (ORNL), Deiterding, Ralf (ORNL), Jakeman, John D. (ORNL), Xiu, Dongbin (ORNL); "Adaptive sparse grids for stochastic collocation on hybrid architectures'" 4/2012, SIAM UQ, Durham, North Carolina
- Archibald, Richard K. (ORNL), Jakeman, John D. (ORNL), Deiterding, Ralf (ORNL), Xiu, Dongbin (ORNL); "Approximation and error estimation in high dimensional stochastic collocation methods on arbitrary sparse samples" 4/2012, SIAM UQ, Durham, North Carolina
- Berrill, Mark A. (ORNL), Chacon, Luis (ORNL), Philip, Bobby (ORNL); "Adaptive Magnetohydrodynamics Simulations with SAMRAI" /2012, TWELFTH COPPER MOUNTAIN CONFERENCE ON ITERATIVE METHODS, Copper, Colorado
- Deiterding, Ralf (ORNL), Wood, Stephen L (University of Tennessee, Knoxville (UTK)); "Parallel FSI simulation of explosions impacting on building structures" 5/2012, Parallel Computational Fluid Dynamics, Atlanta, Georgia
- Evans, Katherine J. (ORNL), Nichols, Jeff ORAU Postdoc (ORNL), Price, Stephen (Los Alamos National Laboratory (LANL)), Salinger, Andy (Sandia National Laboratories (SNL)), Worley, Patrick H. (ORNL); "Nonlinearly consistent continent-scale ice sheet simulations " 10/2011, WCRP: Climate Research in Service to Society, Denver, Colorado
- Kora, Guruprasad H. (ORNL), Holladay, Susan K. (ORNL), Karpinets, Tatiana V. (ORNL), Syed, Mustafa H. (ORNL), Schadt, Christopher Warren (ORNL), Uberbacher, Edward C. (ORNL), Doktycz, Mitchel John (ORNL); "Plant-Microbe Interfaces: Dynamic data analytics through integrated knowledgebase" 2/2012, 2012 Genomic Science Contractors-Grantee Meeting, Bethesda, Maryland
- Maltrud, Matthew E. (Los Alamos National Laboratory (LANL)), McClean, Julie L. (Scripps Institute of Oceanography), Bader, David C. (ORNL), Evans, Katherine J. (ORNL); "Fully-Coupled Fine-Resolution CCSM Simulations: A Prototype and Advancements." 10/2011, World Research Climate Programme, Denver, Colorado
- Martin, Michael (Texas A&M University), Mukherjee, Partha P. (ORNL), Pannala, Sreekanth (ORNL), Allu, Srikanth (ORNL), Ranjan, Devesh (Texas A&M University), Turner, John A. (ORNL); "Electrochemical and Transport Behavior of Lithium Ion Battery 3-D Electrode Architectures" 5/2012, ECS Meeting, Seattle, Washington

Publications/Presentations

- Pernice, Michael (Idaho National Laboratory (INL)), Philip, Bobby (ORNL); "3D Structured Adaptive Mesh Renement and Multilevel Preconditioning for Non-Equilibrium Radiation Diusion" 3/2012, Twelfth Copper Mountain Conference On Iterative Methods, Copper Mountain, Colorado
- Philip, Bobby (ORNL), Clarno, Kevin T. (ORNL), Sampath, Rahul S. (ORNL), Berrill, Mark A. (ORNL), Allu, Srikanth (ORNL); "A Jacobian Free Newton Krylov Method With Multilevel Block Preconditioning for Multi-Domain Quasistatic Thermomechanics" 3/2012, Twelfth Copper Mountain Conference On Iterative Methods, Copper Mountain, Colorado
- Philip, Bobby (ORNL), Clarno, Kevin T. (ORNL), Sampath, Rahul S. (ORNL), Berrill, Mark A. (ORNL), Allu, Srikanth (ORNL), Dilts, Gary (Los Alamos National Laboratory (LANL)); "The Advanced Multi-Physics (AMP) Package" 3/2012, Twelfth Copper Mountain Conference On Iterative Methods, Copper Mountain, Colorado
- Sampath, Rahul S. (ORNL), Philip, Bobby (ORNL), Simunovic, Srdjan (ORNL); "Recursive Schur Decomposition" 2012, Copper Mountain Conference on iterative Methods, Copper Mountain, Colorado
- Wong, Kwai (ORNL), Huang, Amy (Chinese University of Hong Kong, China), Wu, Watson (Chinese University of Hong Kong, China); "OUT-OF-CORE ALGORITHMS FOR DENSE MATRIX FACTORIZATION ON GPGPU" 2/2012, SIAM Conference on Parallel Processing for Scientific Computing, Savannah, Georgia
- Reuter, Matthew G. (ORNL); "Becoming a Ghost Buster" 2012

Book Chapters and Articles

- Beste, Ariana (ORNL), Attalla, Moetaz (CSIRO ICT Center, Australia), Jackson, Phil (CSIRO ICT Center, Australia); "The Kinetics and Thermodynamics of CO2 Capture by Aqueous Ammonia Derived Using Meta-GGA Density Functional Theory and Wavefunction-Based Model Chemistry Methods" 2012
- Meunier, V. (Rensselaer Polytechnic Institute (RPI)), Sumpter, Bobby G. (ORNL), Girao, Eduardo Costa (Universidade Federal do Piaui); "Modeling and simulation of electron transport at the nanoscale: illustrations in low-dimensional carbon nanostructures" 6/2012
- Worley, Patrick H. (ORNL), Vertenstein, Mariana (National Center for Atmospheric Research (NCAR)), Craig, Anthony (National Center for Atmospheric Research (NCAR)); "Community Climate System Model" 9/2011

Journal Articles

- 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, pgs 2866-2888, vol. 436, issue 8
- D'Azevedo, Ed F. (ORNL), Nintcheu Fata, Sylvain (ORNL); "On the effective implementation of a boundary element code on graphics processing units using an out-of-core LU algorithm" Engineering Analysis with Boundary Elements 8/2012, pgs 1246-1255, vol. 36, issue 8
- Dennis, John (National Center for Atmospheric Research (NCAR)), Vertenstein, Mariana (National Center for Atmospheric Research (NCAR)), Worley, Patrick H. (ORNL), Mirin, Arthur A. (Lawrence Livermore National Laboratory (LLNL)), Craig, Anthony (National Center for Atmospheric Research (NCAR)), Jacob, Robert L. (Argonne National Laboratory (ANL)), Mickelson, Sheri A. (Argonne National Laboratory (ANL)); "Computational Performance of Ultra-High-Resolution Capability in the Community Earth System Model" International Journal of High Performance Computing Applications 2/2012, pgs 5-16, vol. 26, issue 1
- Endeve, Eirik (ORNL), Cardall, Christian Y. (ORNL), Budiardja, Reuben D. (ORNL), Beck, Sam (University of Tennessee, Knoxville (UTK)), Bejnood, Alborz (ORNL), Toedte, Ross J. (ORNL), Blondin, J. M. (North Carolina State University), Mezzacappa, Anthony (ORNL); "Turbulent Magnetic Field Amplification from

Publications/Presentations (continued)

Spiral SASI Modes: Implications for Core-Collapse Supernovae and Proto-Neutron Star Magnetization" Astrophysical Journal 5/2012, pgs 1-28, vol. N/A, issue 751

- Gent, Peter (National Center for Atmospheric Research (NCAR)), Donner, Leo (NOAA Geophysical Fluid Dynamics Laboratory (GFDL), Princeton, NJ), Holland, Markia (National Center for Atmospheric Research (NCAR)), Hunke, Elizabeth (Los Alamos National Laboratory (LANL)), Jayne, Steve (Woods Hole Oceanographic Institution (WHOI), Woods Hole, MA), Lawrence, David M. (National Center for Atmospheric Research (NCAR)), Neale, Richard B. (National Center for Atmospheric Research (NCAR)), Rasch, Philip J. (Pacific Northwest National Laboratory (PNNL)), Vertenstein, Mariana (National Center for Atmospheric Research (NCAR)), Worley, Patrick H. (ORNL), Yang, Zong-Liang (University of Texas, Austin), Zhang, Minghua (Stony Brook University (SUNY)); "The Community Climate System Model Version 4" Journal of Climate 10/2011, pgs 4973-4991, vol. 24, issue 19
- Gray, Leonard J. (ORNL), Garzon, Maria (University of Oviedo), Sethian, James A. (Lawrence Berkeley National Laboratory (LBNL)); "Axisymmetric boundary integral formulation for a two fluid system" International Journal for Numerical Methods in Engineering 6/2012, pgs 1124-1134, vol. 69, issue 6
- 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, pgs 378-400, vol. 12, issue 2
- Jakowski, Jacek (ORNL), Irle, Stephan (ORNL), Morokuma, Keiji (ORNL), Sumpter, Bobby G. (ORNL); "Modeling Charge Transfer in Fullerene Collisions via Real-Time Electron Dynamics" Journal of Physical Chemistry Letters 5/2012, pg 1536, vol. 3
- Kotas, Charlotte W. (ORNL), Rogers, Peter (Georgia Institute of Technology), Yoda, Minami (Georgia Institute of Technology); "Acoustically Induced Streaming Flows near a Model Cod Otolith and their Potential Implications for Fish Hearing" Journal of the Acoustical Society of America 8/2011, pgs 1049-1059, vol. 130, issue 2
- Kumar, Rajeev (ORNL), Sumpter, Bobby G. (ORNL), Kilbey, II, S Michael (ORNL); "Charge regulation and local dielectric function in planar polyelectrolyte brushes" Journal of Chemical Physics 6/2012, vol. 136
- Lashuk, Ilya (Lawrence Livermore National Laboratory (LLNL)), Chandramowlishwaran, Aparna (Georgia Institute of Technology), Langston, Harper (Georgia Institute of Technology), Nguyen, Tuan-Anh (Georgia Institute of Technology), Sampath, Rahul S. (ORNL), Shringarpure, Aashay (Georgia Institute of Technology), Vuduc, Richard (Georgia Institute of Technology), Ying, Lexing (University of Texas, Austin), Zorin, Denis (New York University), Biros, George (University of Texas, Austin); "A Massively Parallel Adaptive Fast Multipole Method on Heterogeneous Architectures" Communications of the ACM 5/2012, pg 101, vol. 55, issue 5
- Morris-cohen, Adam J (Northwestern University, Evanston), Vasilenko, Vladislav (Northwestern University, Evanston), Amin, Victor A (Northwestern University, Evanston), Reuter, Matthew G. (ORNL), Weiss, Emily A (Northwestern University, Evanston); "Model for Adsorption of Ligands to Colloidal Quantum Dots with Concentration-Dependent Surface Structure" ACS Nano 1/2012, pgs 557-565, vol. 6, issue 1
- Nintcheu Fata, Sylvain (ORNL); "Treatment of domain integrals in boundary element methods" Applied Numerical Mathematics 6/2012, pgs 720-735, vol. 62, issue 6
- Petrova, Tetyana (Jackson State University), Odbadrakh, Khorgolkhuu (ORNL), Fuentes-Cabrera, Miguel A. (ORNL), Lewis, James (West Virginia University), Leszczynski, Jerzy (Computational Center for Molecular Structure and Interactions, Jackson, MS); "Molecular simulations of adsorption of RDX and TATP on IRMOF-1(Be) " Journal of Molecular Modeling 6/2012, pgs 3363-3378, vol. 18, issue 7
- Philip, Bobby (ORNL), Chartier, Dr Timothy (Davidson College); "Adaptive Algebraic Smoothers" Journal of Computational and Applied Mathematics 3/2012, pgs 2277-2297, vol. 236, issue 9

Publications/Presentations (continued)

- Qiao, Rui (Clemson University), Meunier, V. (Rensselaer Polytechnic Institute (RPI)), Huang, Jingsong (ORNL), Wu, Peng (ORNL), Sumpter, Bobby G. (ORNL); "Voltage Dependent Charge Storage Modes and Capacity in Subnanometer Pores" Journal of Physical Chemistry Letters 6/2012, pgs 1732, vol. 3
- Reuter, Matthew G. (ORNL), Hersam, Mark C. (Northwestern University, Evanston), Seideman, Tamar (Northwestern University, Evanston), Ratner, Mark A. (Northwestern University, Evanston); "Signatures of Cooperative Effects and Transport Mechanisms in Conductance Histograms" Nano Letters 5/2012, pgs 2243-2248, vol. 12, issue 5
- Reuter, Matthew G. (ORNL), Seideman, Tamar (Northwestern University, Evanston), Ratner, Mark A. (Northwestern University, Evanston); "Molecular Conduction through Adlayers: Cooperative Effects can Help or Hamper Electron Transport" Nano Letters 11/2011, pg 4693, vol. 11, issue 11
- Sumpter, Bobby G. (ORNL), Meunier, Vincent (ORNL); "Can Computational Approaches Aid in Untangling the Inherent Complexity of Practical Organic Photovoltaic Systems?" Journal of Polymer Science, Part B: Polymer Physics 5/2012
- Sumpter, Bobby G. (ORNL), Meunier, Vincent (ORNL), Terrones Maldonado, Humberto (ORNL), Terrones Maldonado, Mauricio (ORNL), Ajayan, Pullikel M (Rice University), Hashim, Daniel (Rice University), Romo Herrera, Jose M. (ORNL), Cullen, David (ORNL), Munoz-Sandoval, Emilio (IPICyT), Smith, David J (Arizona State University), Vajtai, Robert (Rice University), Roy, Ajit K. (ORNL), Ganguli, Sabyasachi (Arizona State University), Kelkhoff, Doug (University of Illinois, Urbana-Champaign), Suttle, Joesph (University of Illinois, Urbana-Champaign), Lezzi, Peter (Rensselaer Polytechnic Institute (RPI)), Hahm, Gwan (Rice University), Narayanan, Narayanan (Rice University); "Covalently bonded three-dimensional carbon nanotube solids via boron induced nanojunctions" Scientific Reports 4/2012, pgs 1-8

ORNL Reports

- Bernholdt, David E. (ORNL); "NEAMS Software Licensing, Release, and Distribution: Implications for FY2013 Work Package Planning" 6/2012
- Bernholdt, David E. (ORNL); "Recommendations for NEAMS Engagement with the NRC: Preliminary Report" 6/2012
- Bernholdt, David E. (ORNL), Allan, Benjamin A. (Sandia National Laboratories (SNL)), Armstrong, Robert C. (Sandia National Laboratories (SNL)), Chavarria-Miranda, Daniel (Pacific Northwest National Laboratory (PNNL)), Dahlgren, Tamara L. (Lawrence Livermore National Laboratory (LLNL)), Elwasif, Wael R. (ORNL), Epperly, Tom (Lawrence Livermore National Laboratory (LLNL)), Foley, Samantha S. (ORNL), Hulette, Geoffrey C. (Sandia National Laboratories (SNL)), Krishnamoorthy, Sriram (Pacific Northwest National Laboratory (PNNL)), Prantl, Adrian (Lawrence Livermore National Laboratory (LLNL)), Panyala, Ajay (Louisiana State University), Sottile, Matthew (Galois, Inc.); "COMPOSE-HPC: A Transformational Approach to Exascale" 4/2012
- Weerapurage, Dinesh P. (ORNL), Sullivan, Blair D. (ORNL), Groer, Christopher S. (ORNL); "Parallel Algorithms for Graph Optimization using Tree Decompositions" 6/2012
- Wood, Stephen L. (ORNL), Deiterding, Ralf (ORNL); "Shock-driven fluid-structure interaction for civil design" 11/2011
- Ang, Jim (Sandia National Laboratories (SNL)), Evans, Katherine J. (ORNL), Geist, Al (ORNL), Heroux, Dr. Michael A (Sandia National Laboratories (SNL)), Hovland, Paul (Argonne National Laboratory (ANL)), Marques, Osni (Lawrence Berkeley National Laboratory (LBNL)), McInnes, Lois (Argonne National Laboratory (ANL)), Ng, Esmond (Lawrence Berkeley National Laboratory (LBNL)), Wild, Stephan (Argonne National Laboratory (ANL)); "Workshop on Extreme-Scale Solvers: Transition to Future Architectures" 4/2012

Publications/Presentations (continued)

Papers in Conference Proceedings

- Allen, Melissa R. (ORNL), Erickson III, David J. (ORNL); "Simplified Parallel Domain Traversal" /2011, International Conference for High Performance Computing, Networking, Storage and Analysis, Seattle, Washington
- Archibald, Richard K. (ORNL), Deiterding, Ralf (ORNL), Hauck, Cory D. (ORNL), Jakeman, John D. (ORNL), Xiu, Dongbin (ORNL); "Approximation and error estimation in high dimensional space for stochastic collocation methods on arbitrary sparse samples" 4/2012, Exascale Research Conference, Portland, Oregon
- Archibald, Richard K. (ORNL), Deiterding, Ralf (ORNL), Jakeman, John D. (ORNL); "Extending adaptive sparse grids for stochastic collocation to hybrid parallel architectures" 1/2012, SciDAC 2011, Denver, Colorado
- Boboila, Simona (Northeastern University), Kim, Youngjae (ORNL), Vazhkudai, Sudharshan S. (ORNL), Desnoyers, Peter (Northeastern University), Shipman, Galen M. (ORNL); "Active Flash: Out-of-core Data Analytics on Flash Storage" 4/2012, Proceedings of the 28th IEEE Conference on Mass Storage Systems and Technologies (MSST 2012), Monterey, California
- Elwasif, Wael R. (ORNL), Bernholdt, David E. (ORNL), Berry, Lee A. (ORNL), Batchelor, Donald B. (ORNL); "Component Framework for Coupled Integrated Fusion Plasma Simulation " 2007, HPC-GECO/CompFrame 2007. and Scientific Computing, Montreal
- Elwasif, Wael R. (ORNL), Norris, Boyana (Argonne National Laboratory (ANL)), Benjamin, Allan A. (Sandia National Laboratories (SNL)), Armstrong, Robert C. (Sandia National Laboratories (SNL)); "Bocca: A Development Environment for HPC Components" 2007, HPC-GECO/CompFrame 2007, Montreal
- Ilsche, Thomas (Technische Universitat Dresden), Schuchart, Joseph (Technische Universitat Dresden), Cope, Joseph (Argonne National Laboratory (ANL)), Kimpe, Dries (Argonne National Laboratory (ANL)), Jones, Terry R. (ORNL), Knuepfer, Andreas (Technische Universitat Dresden), Iskra, Kamil (Argonne National Laboratory (ANL)), Ross, Robert (Argonne National Laboratory (ANL)), Nagel, Wolfgang E. (Technische Universitat Dresden), Poole, Stephen W. (ORNL); "Enabling Event Tracing at Leadership-Class Scale through I/O Forwarding Middleware" 6/2012, The 21 International ACM Symposium on High-Performance Parallel and Distributed Computing (HPDC 2012), Delft
- Keller, Rainer (Universitat Stuttgart), Graham, Richard L. (ORNL); "Characteristics of the Unexpected Message Queue of MPI applications" 2010, EuroMPI 2010, Stuttgart
- Kotas, Charlotte W. (ORNL), Barhen, Jacob (ORNL); "Singular value decomposition utilizing parallel algorithms on graphical processors" 2011, OCEANS '11 MTS/IEEE KONA, Waikoloa, Hawaii
- Lifflander, Jonathan (University of Illinois, Urbana-Champaign), Miller, Phil (University of Illinois, Urbana-Champaign), Venkataraman, Ramprasad (University of Illinois, Urbana-Champaign), Arya, Anshu (University of Illinois, Urbana-Champaign), Jones, Terry R. (ORNL), Kale, Laxmikant V (University of Illinois, Urbana-Champaign); "Dense LU Factorization on Multicore Supercomputer Nodes" 5/2012, 26th IEEE International Parallel & Distributed Processing Symposium (IEEE IPDPS 2012), Shanghai
- Rabinovitz, Ishai (Mellanox Technologies, Inc.), Shamis, Pavel (ORNL), Graham, Richard L. (ORNL), Bloch, Noam (Mellanox Technologies, Inc.), Shainer, Gilad (Mellanox Technologies, Inc.); "Network Offoaded Hierarchical Collectives Using ConnectX-2's CORE-Direct Capabilities" 2010, EuroMPI 2010, Stuttgart
- Roth, Philip C. (ORNL), Vetter, Jeffrey S. (ORNL); "Improving Programmer Productivity on Heterogeneous GPU Computing Systems by Broadening and Strengthening the Tools Ecosystem" 4/2012, DOE Exascale Research Conference, Portland, Oregon
- Sun, Yanhua (University of Illinois, Urbana-Champaign), Zheng, Gengbin (University of Illinois, Urbana-Champaign), Olson, Ryan M (Cray, Inc.), Jones, Terry R. (ORNL), Kale, Laxmikant V (University of

Illinois, Urbana-Champaign); "Title A uGNI-Based Asynchronous Message-driven Runtime System for Cray Supercomputers with Gemini Interconnect" 5/2012, 26th IEEE International Parallel & Distributed Processing Symposium (IEEE IPDPS 2012), Shanghai

- Wang, Chao (ORNL), Vazhkudai, Sudharshan S. (ORNL), Ma, Xiaosong (ORNL), Meng, Fei (ORNL), Kim, Youngjae (ORNL), Engelmann, Christian (ORNL); "NVMalloc: Exposing an Aggregate SSD Store as a Memory Partition in Extreme-Scale Machines" 5/2012, Proceedings of the 26th IEEE Intl Parallel & Distributed Processing Symposium (IPDPS 2012), Sanghai
- Worley, Patrick H. (ORNL), Craig, Anthony (National Center for Atmospheric Research (NCAR)), Dennis, John (National Center for Atmospheric Research (NCAR)), Mirin, Arthur A. (Lawrence Livermore National Laboratory (LLNL)), Taylor, Mark (Sandia National Laboratories (SNL)), Vertenstein, Mariana (National Center for Atmospheric Research (NCAR)); "Performance of the Community Earth System Model" 11/2011, International Conference for High Performance Computing, Networking, Storage and Analysis (SC11), Seattle, Washington
- Wu, Qishi (ORNL), Zhu, Mengxia (ORNL), Rao, Nageswara S. (ORNL); "System Design for On-line Distributed Computational Visualization and Steering" 2006, International Conference on E-learning and Games, Hangzhou
- Yu, Li (Illinois Institute of Technology), Zheng, Ziming (Illinois Institute of Technology), Lan, Zhiling (Illinois Institute of Technology), Jones, Terry R. (ORNL), Brandt, Jim (Sandia National Laboratories (SNL)), Gentile, Ann (Sandia National Laboratories (SNL)); "Filtering log data: finding the needles in the haystack" 6/2012, 42nd IEEE/IFIP International Conference on Dependable Systems and Networks (DSN 2012), Boston, Massachusetts
- D'Azevedo, Ed F. (ORNL), Hill, Judith C. (ORNL); "Parallel LU Factorization on GPU cluster" Procedia Computer Science 2012, International Conference on Computational Science, Omaha, Nebraska

Presentation Material - Conference

- Allu, Srikanth (ORNL), Pannala, Sreekanth (ORNL), Mukherjee, Partha P. (ORNL), Philip, Bobby (ORNL), Turner, John A. (ORNL); "Development of single domain framework to model 3D Li-Ion intercalation batteries using the Advanced Multi Physics (AMP) package" Copper Mountain Conference on Iterative Methods 2012, Copper Mountain, Colorado
- Baker, Christopher G. (ORNL), Gallivan, Dr. Kyle A (Florida State University), Van Dooren, Dr. Paul (Universite Catholique de Louvain); "Incremental Methods for Computing Extreme Singular Subspaces" SIAM Conference on Applied Linear Algebra 2012, Valencia
- Baker, Christopher G. (ORNL), Heroux, Dr. Michael A (Sandia National Laboratories (SNL)); "An Overview of the Trilinos Project" European Seminar on Computing, Pilsen
- Branstetter, Marcia L. (ORNL), Jitendra Kumar (ORNL), Peter E. Thornton (ORNL), Michele M. Thornton (ORNL), “High Resolution Surface Weather Forcing Dataset for CLM”, 17th Annual CESM Workshop, Breckenridge, CO, June 18-21, 2012
- Elwasif, Wael R. (ORNL), Bernholdt, David E. (ORNL), Harrison, Robert J. (ORNL); "High Productivity Language Systems: Next-Generation Petascale Programming" SC07 - Supercomputing 2007, Reno, Nevada
- Guy, Robert (University of California, Davis), Philip, Bobby (ORNL); "A multigrid method for the coupled implicit immersed boundary equations" 10th WORLD CONGRESS ON COMPUTATIONAL MECHANICS (WCCM 2012), Sao Paulo
- Guy, Robert (University of California, Davis), Philip, Bobby (ORNL); "A multigrid method for the coupled implicit immersed boundary equations" The Second International Conference on Scientific Computing, Nanjing

Publications/Presentations (continued)

- Guy, Robert (University of California, Davis), Philip, Bobby (ORNL); "A multigrid method for the coupled implicit immersed boundary equations" Society for Engineering Science Annual Meeting, Chicago, Illinois
- Guy, Robert (University of California, Davis), Philip, Bobby (ORNL); "A multigrid method for the coupled implicit immersed boundary equations" SIAM Annual meeting 2010, Pittsburgh, Pennsylvania
- Ilsche, Thomas (Technische Universitat Dresden), Schuchart, Joseph (Technische Universitat Dresden), Cope, Joseph (Argonne National Laboratory (ANL)), Kimpe, Dries (Argonne National Laboratory (ANL)), Jones, Terry R. (ORNL), Knuepfer, Andreas (Technische Universitat Dresden), Iskra, Kamil (Argonne National Laboratory (ANL)), Ross, Robert (Argonne National Laboratory (ANL)), Nagel, Wolfgang E. (Technische Universitat Dresden), Poole, Stephen W. (ORNL); "Enabling Event Tracing at Leadership-Class Scale through I/O Forwarding Middleware (Poster)" The 21 International ACM Symposium on High-Performance Parallel and Distributed Computing (HPDC 2012), Delft
- Ilsche, Thomas (Technische Universitat Dresden), Schuchart, Joseph (Technische Universitat Dresden), Cope, Joseph (Argonne National Laboratory (ANL)), Kimpe, Dries (Argonne National Laboratory (ANL)), Jones, Terry R. (ORNL), Knuepfer, Andreas (Technische Universitat Dresden), Iskra, Kamil (Argonne National Laboratory (ANL)), Ross, Robert (Argonne National Laboratory (ANL)), Nagel, Wolfgang E. (Technische Universitat Dresden), Poole, Stephen W. (ORNL); "Enabling Event Tracing at Leadership-Class Scale through I/O Forwarding Middleware" The 21 International ACM Symposium on High-Performance Parallel and Distributed Computing (HPDC 2012), Delft
- Kartsaklis, Christos (ORNL), Hernandez, Oscar R. (ORNL), Hsu, Chung-Hsing (ORNL), Ilsche, Thomas (Technische Universitat Dresden), Joubert, Wayne (ORNL), Graham, Richard L. (ORNL); "HERCULES: A PATTERN DRIVEN CODE TRANSFORMATION SYSTEM" IPDPSW 2012, Shanghai
- Kent, Paul R. C.; "A Gentle Introduction to Electronic Structure Theory", EFRC Summer School on Defects, Deformation and Damage in Structural Materials, June 2012, Knoxville, TN
- Li, Dong (ORNL), Vetter, Jeffrey S. (ORNL), Marin, Gabriel (ORNL), McCurdy, Collin B. (ORNL), Cira, Christian (Auburn University, Auburn, Alabama), Liu, Zhuo (Auburn University, Auburn, Alabama), Yu, Weikuan (ORNL); "Identifying Opportunities for Byte-Addressable Non-Volatile Memory in Extreme-Scale Scientific Applications" IPDPS, Shanghai
- Maier, Thomas A. (ORNL) "Superconductivity in heterostructures and systems with nanoscale charge inhomogeneities: Numerical studies of Hubbard models", CECAM workshop, June 2012, Lausanne, Switzerland
- Nintcheu Fata, Sylvain (ORNL); "Domain integrals in the BEM" NSF Workshop on the BEM: Bridging Education and Industrial Applications, Minneapolis, Minnesota
- Pannala, Sreekanth (ORNL), Turner, John A. (ORNL), Mukherjee, Partha P. (ORNL), Allu, Srikanth (ORNL), Simunovic, Srdjan (ORNL), Elwasif, Wael R. (ORNL), Bernholdt, David E. (ORNL); "Open Architecture Software for CAEBAT" US DOE Hydrogen and Vehicle Technologies Program Annual Merit Review and Peer Evaluation, Washington D.C., District of Columbia
- Philip, Bobby (ORNL); "3D Structured Adaptive Mesh Refinement and Multilevel Preconditioning for Non-Equilibrium Radiation Diusion" SIAM South Eastern Atlantic Conference, Huntsville, Alabama
- Philip, Bobby (ORNL); "The Advanced Multi-Physics (AMP) Package" Twelfth Copper Mountain Conference On Iterative Methods, Copper Mountain, Colorado
- Philip, Bobby (ORNL), Clarno, Kevin T. (ORNL), Sampath, Rahul S. (ORNL), Berrill, Mark A. (ORNL), Dilts, Gary (Los Alamos National Laboratory (LANL)), Hamilton, Steven P. (ORNL), Allu, Srikanth (ORNL), Barai, Pallab (ORNL), Banfield, James E. (ORNL); "A Jacobian Free Newton Krylov Method With

Publications/Presentations (continued)

Multilevel Block Preconditioning for Multi-Domain Quasistatic Thermomechanics" Twelfth Copper Mountain Conference On Iterative Methods, Copper Mountain, Colorado

- Philip, Bobby (ORNL), Wang, Zhen (ORNL), Rodriguez Rodriguez, Manuel G. (ORNL), Berrill, Mark A. (ORNL), Pernice, Michael (Idaho National Laboratory (INL)); "3D Structured Adaptive Mesh Refinement and Multilevel Preconditioning for Non-Equilibrium Radiation Diffusion" ASTRONUM 2012, Kona-Kailua, Hawaii
- Sullivan, Blair D. (ORNL), Groer, Christopher S. (ORNL); "Are Tree Decompositions Practical for Large-Scale Computing?" ICIAM 2011, Vancover
- Sullivan, Blair D. (ORNL), Groer, Christopher S. (ORNL), Mahoney, M (Stanford University), Adcock, Aaron (Stanford University), Shojaie, Ali (University of Michigan), Lenaric, Alan (University of North Carolina, Chapel Hill); " Tree Decompositions and Complex Networks" SAMSI Complex Networks Transitions Workshop, Raleigh-Durham, North Carolina
- Sumpter, Bobby G. (ORNL); "Guiding the Design of Functional Materials for Energy S&T" Workshop on Opportunities for Accelerating Neutron Data Analysis, Oak Ridge, Tennessee
- Sumpter, Bobby G. (ORNL); "Nanostructured Soft-Matter Materials" Recent Advances in Materials Physics Symposium, Raleigh, North Carolina
- Worley, Patrick H. (ORNL); "Capturing Computer Performance Variability in CESM Experiments" 17th Annual Community Earth System Model Workshop, Breckenridge, Colorado
- Worley, Patrick H. (ORNL), Evans, Katherine J. (ORNL), Lipscomb, William (Los Alamos National Laboratory (LANL)), Nichols, Jeff ORAU Postdoc (ORNL), Price, Stephen (Los Alamos National Laboratory (LANL)), Salinger, Andy (Sandia National Laboratories (SNL)); "Parallel implementation and performance of SEACISM version of CISM" 17th Annual Community Earth System Model Workshop, Breckenridge, Colorado

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

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

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

OAK RIDGE National Laboratory