

Events

1st Annual Postdoctoral Symposium at ORNL (July 18)
The Oak Ridge National Laboratory is revamping the entire postdoctoral program as a strategic initiative to foster the next generation of world-class researchers. As part of this process, the Oak Ridge Postdoctoral Association (ORPA) has been formed to facilitate the holistic development of postdoctoral researchers. ORNL attracts the best talent from all over the world. Not only does ORPA help these scholars in settling down in East Tennessee, it also provides information resources, workshops, tutorials, and various other developmental tools thereby facilitating social, international, career development, and research needs to create a vibrant research community.

The Wigner and Weinberg Fellows in collaboration with the Oak Ridge Postdoctoral Association are organizing the 1st Annual Postdoctoral Symposium at ORNL on July 18, 2013. This is the first event of its kind. ORNL's postdoctoral researchers will present posters and talks about their current research in the day-long event. The symposium will open with remarks by Dr. Thom Mason, Laboratory Director, and will have a keynote session presented by Dr. Ramamoorthy Ramesh, Deputy Director for Science and Technology. Awards for outstanding oral and poster presentations will be presented.

Contact Matt Reuter (reutermg@ornl.gov) for more information.



Highlights

Nuclear Mass Dataset Dissemination and Analysis with the Nuclear Masses Toolkit and nuclearmasses.org

ORNL Team Members: Michael Smith (PI), Eric J. Lingerfelt, Caroline D. Nesaraja, and Chris Smith

A knowledge of the masses of subatomic nuclei forms a crucial foundation for research in basic and applied nuclear science, as well as in astrophysics. New accelerator facilities and new detection systems have enabled researchers around the world to make more, and much more precise, nuclear mass measurements. In late 2012, a new Atomic Mass Evaluation was released, the first in a decade, that included all of this new information. However, the dissemination of these new masses (as an 850-page paper or as one enormous electronic table) has limited utility for researchers. Our Nuclear Masses Toolkit (NMT) provides the only online dissemination of these new masses whereby a ready comparison can be made with older masses and with the predictions of over 13 different theoretical mass models.

Freely available at the website nuclearmasses.org, the NMT enables research scientists and non-experts the ability to share, visualize and analyze nuclear mass information in a robust and intuitive way. Once registered, Users can upload mass datasets, store them, and share them with colleagues as well as compare mass datasets with ones from peer-reviewed research. The NMT's suite of visualization tools allows Users to quickly and easily create highly customized

data views of several quantities and their differences when compared to other datasets. The data views not only include 1D plots but also interactive 2D plots on the chart of the nuclides that compare values such as mass excess, Q-values, and separation energies. Datasets may also be analyzed by average RMS differences and RMS difference as a function of atomic number, neutron number, and mass number. In addition to the capabilities offered by the NMT, the nuclearmasses.org website provides the scientific community detailed information and links concerning theoretical and experimental mass datasets. It also creates a mechanism for Users to inform the community of their latest mass models, measurements, and software tools.

This work was initially funded through an ORNL Seed Proposal in 2008 and is currently funded by the US Nuclear Data Program of the Office of Nuclear Physics in the U.S. Department of Energy Office of Science.

New Version of C3 Released

ORNL Team Members: Mike Brim, John Mugler, Geoffroy Vallee, Wesley Bland, and Thomas Naughton

A new version of the Cluster Command Control (C3) tools has been released. The C3 tools are used as a core piece of the OSCAR cluster management suite, which has been updated to support the latest Ubuntu Linux distribution. These updated cluster tools are used internally by members of Computer Science Research to maintain group machines.

Highlights (continued)

They are also used stand-alone by a variety of users from industry, academia and laboratories.

C3 is a suite of cluster tools developed at ORNL that are useful for both administration and application support. The suite includes tools for cluster-wide command execution, file distribution/gathering, process termination and with proper privileges remote node shutdown. The tools can be installed for general system use or run from a user's home directory. By default, the tools use SSH to connect to the remote machines and support a rich set of options for cluster or multi-cluster setup.

OSCAR is a cluster installation and management suite that can be used to setup an system with common HPC software, e.g., job schedulers, message passing libraries, etc. The latest version of the suite was extended to support lab approved Linux and system management policies. This enhanced version of OSCAR was used to deploy two clusters maintained by CSR members: HAL9000 and SAL9000. These platforms are used for research and development of HPC system software and resilience research.

ORNL is a founding member of the OSCAR project and has maintained a leadership role in the development and maintenance of the suite over the past decade. The C3 tools were first developed at ORNL in 2000. The C3 project was started by Stephen Scott and Brian Luethke as the lead developers. In addition to community patches and bug reports, over the years several individuals have contributed to the development and maintenance of C3, to include: Mike Brim, John Mugler, Geoffroy Vallee, Wesley Bland, and Thomas Naughton.

For more information about these tools and cluster platforms, see:

- C3 Cluster tools (<http://www.csm.ornl.gov/torc/c3/>)
- OSCAR Cluster suite (<http://oscar.openclustergroup.org/>)
- Systems Research Team Projects Page (http://www.csm.ornl.gov/srt/projects_index.html)

Electronic control over molecular self-assembly and polymerization

ORNL Team Members: Qing Li, Chengbo Han, Bobby Sumpter, Wenchang Lu, Jerry Bernholc, Petro Maksymovych, Miguel Fuentes-Cabrera, and Minghu Pan

CSMD and CNMS researchers Qing Li, Jonathan Owens, Chengbo Han, Bobby G. Sumpter, Wenchang Lu, Jerry Bernholc, Vincent Meunier, Petro Maksymovych, Miguel Fuentes-Cabrera, and Minghu Pan have demonstrated a non-thermal, electron-induced approach to the self-assembly of phenylacetylene molecules on gold that allows for a previously unachievable attachment of the molecules to the surface through the alkyne group and further controllable surface-coordinated linear polymerization of long-chain poly(phenylacetylenyl)s that are self-organized into a “circuit-board” pattern.

Self-assembly (the process in which a disordered system of pre-existing components forms an organized structure or pattern as a consequence of specific, local interactions among the components themselves, without external direction) is the key to bottom-up design of molecular devices, because the nearly atomic-level control is very difficult to realize in a top-down, e.g., lithographic approach. Self-assembly of the molecular chains previously achieved using thermally driven processes, as opposed to electronic control in this work, leads to defects and largely uncontrolled surface packing. To enable electronic devices, it is essential to control defects at the interface (the interface makes or breaks a device), which is one of the advantages of an all-electronic control over self-assembly and polymerization.

Self-Organized and Cu-Coordinated Surface Linear Polymerization, Qing Li, Jonathan Owens, Chengbo Han, Bobby G. Sumpter, Wenchang Lu, Jerry Bernholc, Vincent Meunier, Petro Maksymovych, Miguel Fuentes-Cabrera, Minghu Pan, Nature Sci. Rep. DOI:10.1038/srep02102 (2013)

Open MPI version 1.7 and 1.7.1 released with Cheetah Framework and Cray XE/XK Support

ORNL Team Members: Pavel Shamis and Manjunath Gorentla Venkata

Open MPI version 1.7 was released with various new features including Cheetah framework and support for Cray XE/XK Systems. The bug fixes to v1.7 was released in the latest minor release version 1.7.1. Open MPI v1.7.1 is now available as a module on Titan.

Cheetah is a framework for implementing collective operations for modern supercomputers, and for various programming models including message passing and global address space models. It is a joint effort of Oak Ridge National Laboratory (ORNL), and Mellanox Technologies. The Cheetah research shaped the features and capabilities of Mellanox's CORE-Direct technology, which is now a part of their products. The ORNL team includes Pavel Shamis and Manjunath Gorentla Venkata, who are both members of Computer Science Research Group.

They, along with researchers and engineers from Mellanox Technologies, built many prototypes before arriving at the current solution. The Cheetah framework released along with Open MPI v1.7 provides an infrastructure for implementing blocking and non-blocking collective communication operations, as well as a reference implementation of Barrier and Broadcast collectives.

Open MPI support for Cray XE/XK was a joint effort of ORNL and Los Alamos National Laboratory (LANL). The ORNL team included Manjunath Gorentla Venkata, and LANL team included two researchers from LANL's HPC group. It is the only available open source implementation of MPI for Cray XE/XK family of systems.

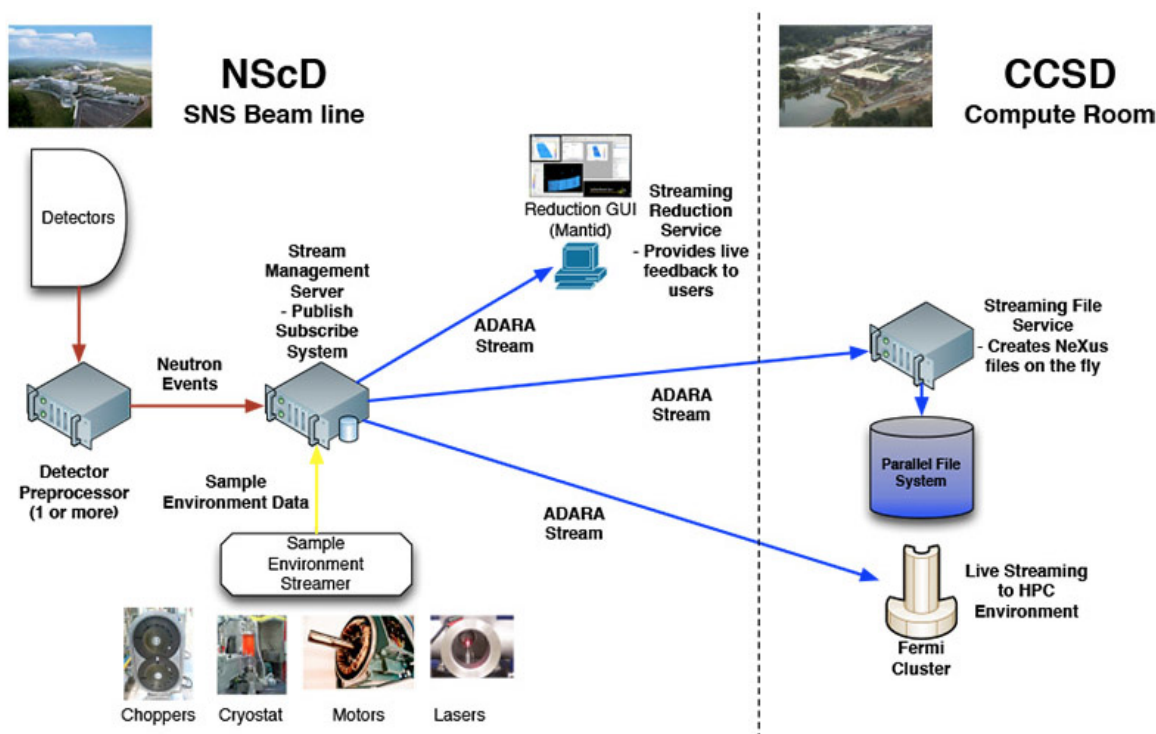
Highlights (continued)

Accelerating Data Acquisition, Reduction, and Analysis (ADARA)

ORNL operates the world's brightest neutron source, the Spallation Neutron Source (SNS). Funded by the US DOE Office of Basic Energy Science, this national user facility hosts hundreds of scientists from around the world, providing a platform to enable break-through research in materials science, sustainable energy, and basic science. OCLF personnel have been engaged to help manage and analyze the large data sets (ranging in size from 100's of gigabytes to over 1 terabyte) generated by the intense pulses of neutrons.

Members of ORNL's Computing and Computational Sciences Directorate (CCSD) and SNS data specialists from the Neutron Data Analysis and Visualization Division have collaborated to successfully complete the Accelerating Data Acquisition, Reduction, and Analysis (ADARA) Lab-Directed Research and Development project to improve the production and analysis of these data sets. The ADARA project has brought together experts in high-performance file systems, parallel processing, cluster configuration and management, data management, and Neutron Science. As a result of the ADARA project, a new data infrastructure was created that enhances users' ability to collect, reduce, and analyze data as it is taken; create data files immediately after acquisition, regardless of size; reduce a data set in seconds after acquisition; and provide the resources for any user to do post-acquisition reduction, analysis, visualization, and modeling without requiring users to be on-site at the SNS facility.

ADARA is currently running on the HYSPEC beam line providing near real-time access to result data sets (both raw event data and reduced data) so that instrument scientists and users now obtain live feedback from their experiments. Moving forward, ADARA will be deployed in production across the beam lines at SNS. Due to the success of the ADARA LDRD, the project has transitioned to operations within the SNS and ongoing development activities are funded as part of ongoing SNS operations. For more information on the ADARA project please contact Galen Shipman (gshipman@ornl.gov).



Galen Shipman (PI), Mark Hagen (co-PI), Thomas Proffen (NDAV Division Director), Ryan Adamson, Blake Caldwell, Stuart Campbell, Lloyd Clonts, David Dillow, Mathieu Doucet, Dave Giles, Melissa Graves-Brook, Gayle Greene, Matthew Gyurgyik, Steven Hartman, Matthew Hermanson, Steve Hicks, Kay Kasemir, Jason Kincl, Scott Koch, James Kohl, Chris Layton, Vickie Lynch, Robert McGreevy, Ross Miller, Sarp Oral, Andre Parizzi, Daniel Pelfrey, Pete Peterson, Doug Reitz, Shelly Ren, Michael Reuter, Charles Roberts, Andrei Savici, Sergey Shpanskiy, Brian Smith, Dale Stansberry, Madhan Sundaram, John Quigley, Carol Tang, Kevin Thach, Tara Thompson, Sudharshan Vazhkudai, Pedro Vicente, Feiyi Wang, Karen White, Barry Winn, Russell Taylor, Marie Yao, Piotr Zolnierczuk

Highlights (continued)

Scaling To A Million Cores And Beyond: Using Light-Weight Simulation to Understand The Challenges Ahead On The Road To Exascale

ORNL Team Member: Christian Engelmann

The path to exascale high-performance computing (HPC) poses several challenges related to power, performance, resilience, productivity, programmability, data movement, and data management. Investigating the performance of parallel applications at scale on future architectures and the performance impact of different architecture choices is an important component of HPC hardware/software co-design. Without having access to future architectures at scale, simulation approaches provide an alternative for estimating parallel application performance on potential architecture choices. As highly accurate simulations are extremely slow and less scalable, different solution paths exist to trade-off simulation accuracy in order to gain simulation performance and scalability.

The Extreme-scale Simulator (xSim) is a performance investigation toolkit that permits running native HPC applications or proxy applications in a controlled environment with millions of concurrent execution threads, while observing application performance in a simulated extreme-scale system for hardware/software co-design. Using a lightweight parallel discrete event simulation (PDES), xSim executes a Message Passing Interface (MPI) application on a much smaller system in a highly oversubscribed fashion with a virtual wall clock time, such that performance data can be extracted based on a processor and a network model with an appropriate simulation scalability/accuracy trade-off. xSim is designed like a traditional performance tool, as an interposition library that sits between the MPI application and the MPI library, using the MPI profiling interface.

The capabilities and usefulness of the xSim toolkit have been recently demonstrated [1] by showing that (a) it scales to 134,217,728 (2^{27}) simulated MPI ranks, each with its own context, on a 960-core Linux cluster (a world record in extreme-scale simulation), (b) different MPI collective communication algorithms could be evaluated on a simulated future-generation system with up to 2,097,152 (2^{21}) simulated MPI ranks using the same cluster, and (c) the scaling properties of a Monte Carlo solver with different architectural parameters could be investigated on a simulated HPC system with up to 16,777,216 (2^{24}) simulated MPI ranks using the same cluster. The results clearly demonstrate that architecture-awareness is key to enable extreme-scale computing. Whether it is collective communication algorithms within the MPI implementation, application scalability limits imposed by Amdahl's law, or energy efficiency trade-offs in hardware, HPC hardware/software co-design is essential to guarantee efficient utilization of future-generation HPC systems.

[1] Christian Engelmann. Scaling To A Million Cores And Beyond: Using Light-Weight Simulation to Understand The Challenges Ahead On The Road To Exascale. Future Generation Computer Systems (FGCS), 2013. Elsevier B.V, Amsterdam, The Netherlands. In press.

Software Releases

SystemBurn 3.1.0

SystemBurn 3.1.0 was released as Open Source on github. This release contains several new features, including:

- The addition of PAPI performance counters
- Support for OpenCL GEMM and memory stress loads
- Support for OpenACC GEMM loads
- A test harness for identifying load combinations that maximize power consumption

The OpenACC standards organization released version 2.0 of the standard at the ICS conference in Leipzig. The specification includes enhancements for performance, portability and programmability. The speedup is derived from new controls over data movement, including better handling of unstructured data and improvements in support for non-contiguous memory. (<http://www.openacc.org/sites/default/files/OpenACC%202%200.pdf>)

XDD 7.0.0 rc24

XDD 7.0.0 rc24 was released to its customers for use in production systems. RC24 includes lockstep functionality that makes it possible to simulate log-structured storage systems and simulate slotted access to storage systems.

HERCULES 2.2 (r278)

HERCULES is an Open64-based, PROLOG-backed, system for program constraint programming and customizable, user-level, transformation formulation. In addition to the core system, it offers a source code base scanner for patterns (hscan) and numerous transformation directives in an F90 compiler (hslf90).

This release features:

- spl: control flow constraints (structured & unstructured).
- spl: array access constraints & use-def constraints.
- language: property clause negation (!) in addition to NaF (-).
- language: subtyping & new type 'block'.
- language: component qualifiers (rhs, then, else).
- language: new aggregator {} (in addition to []) for tree-wide constraint propagation.
- language: 'flush' directive to intercept the breadth-first emission of constraints.
- language: new keyword 'commutative'.
- language: new pattern generation mode 'slist'.
- sdk: the fact importation infrastructure has been externalized.
- hdp: precision relaxation for floats, trap unbound identifiers.

HERCULES is available as a module on the 'yona' and 'chester' NCCS systems.

New Funding

MCREX

ORNL Team Members: Thomas Evans, Steven Hamilton, Wayne Joubert, and Christian Engelmann

The MCREX - Monte Carlo Resilient Exascale Solvers project has been funded by the DOE's Office of Advanced Scientific Computing Research under the Resilient Extreme-Scale Solvers (RX-Solvers) program. The project is lead by Thomas M. Evans from the Radiation Transport Group in ORNL's Reactor and Nuclear Systems Division. The other investigators are Steven P. Hamilton from the Radiation Transport Group, Wayne Joubert from ORNL's Scientific Computing Group, Christian Engelmann from ORNL's Computer Science Research Group, and Michele Benzi from Emory University's Department of Mathematics and Computer Science.

The next generation of computational science applications will require numerical solvers that are capable of high performance on proposed exascale platforms. In order to meet this goal, solvers must be resilient to soft and hard failures, provide high concurrency on heterogeneous hardware configurations, and retain numerical accuracy and efficiency. In light of these requirements, a natural avenue of inquiry would be to adapt the current stable of numerically efficient solvers to this new high-performance computing (HPC) regime. However, an alternative approach is to investigate different classes of algorithms that can address issues of resiliency naturally. This project investigates new stochastic methods for solving linear systems, otherwise termed Monte Carlo Resilient Exascale (MCREX) solvers. The family of methods builds on the sequential Monte Carlo work of Halton, 1962. While showing significant promise, this class of solvers has not made inroads into the broader computational science community. Our initially developed methods use Monte Carlo to accelerate a fixed-point iteration. Therefore, they are called Monte Carlo Synthetic Acceleration (MCSA). Preliminary work using MCSA has demonstrated that they are at least as efficient as Jacobi-preconditioned Conjugate Gradient (PCG) on sparse, SPD systems. These initial results demonstrate that, because MCSA does not require symmetry or positive definiteness, very good efficiency could be attained on non-symmetric systems, thus making MCSA an ideal solver in non-linear Newton schemes. Furthermore, Monte Carlo methods have the benefit of addressing resiliency in a natural way; soft errors can be treated as high variance samples and lost histories from processor failures can be easily discarded without affecting the quality of the solution.

CSC110

ORNL Team Member: Terry Jones

A new Advanced Leadership Computing Challenge (ALCC) allocation will be used by the HPC Colony project to evaluate innovations that are leading to more sophisticated system software. CSMD Computer Scientist and Project PI Terry Jones explains that the current trend among the most powerful computers is toward much more parallelism and more machine complexity. This in turn can potentially lead to a greater challenge for would-be users of machines like Titan. "We're doing research to develop smart system software that adapts the resources of complex machines like Titan automatically to any application" explained Jones. "Today, the most successful simulation teams frequently have a strong understanding of computer science and the machine architecture. That's a pretty high barrier that we would like to reduce as much as possible."

The allocation, CSC110, provides 3 million hours on Titan to perform the necessary experiments to conduct the system software R&D. "Working at a place that has the worlds most powerful computer for open science is an incredible benefit to those who are interested in High Performance Computing, but the benefit would be much less meaningful without programs like the Director's Discretion program", said Jones. "This will allow us to carefully examine how 'on-paper' theory agrees with actual implementation measurements. As with any study, sometimes there are surprises which can lead to further breakthroughs. We are looking forward to the fruits of this allocation"

The mission of the ALCC is to provide an allocation program for projects of interest to the Department of Energy (DOE) with an emphasis on high-risk, high-payoff simulations in areas directly related to the DOE mission and for broadening the community of researchers capable of using leadership computing resources.



New Faces in CSMD



Summer Students

CSMD is proud to host close to 70 student interns this summer. Each student is assigned to a STEM research mentor to work on a project of interest to the student, the student's professor(s), and the ORNL researcher. The students consist of undergraduate, masters and PhD levels from top Universities across the U.S. The students are a part of three primary Internship Programs available at ORNL; the Research Alliance for Math and Science Program, sponsored by the Office of Advanced Scientific Computing Researcher; the Science Undergraduate Laboratory Internship (SULI) Program, sponsored and managed by the DOE Office of Science's, Office of Workforce Development for Teachers and Scientists (WDTS); and the Higher Education Research Experiences Program funded by CSMD programmatic funds. CSMD is also currently hosting several local high school interns as part of the Oak Ridge High School Math Thesis Program and the Appalachian Regional Commission (ARC)/Oak Ridge National Laboratory (ORNL) High School Summer Math-Science-Technology Institute.

Additionally, the Predictive Methods Group (PMG) in CSMD is pleased to introduce the ORACLE Graduate Internship Program. The ORACLE Program consists of graduate students that are beginning their career in the fields of mathematics and statistics. These participants will work to produce the fundamental understanding and algorithms needed to maximize the knowledge that can be gained from world-class leadership computing.

The CSMD summer students have the opportunity to meet and collaborate with other staff researchers within CSMD as well as around the laboratory. The students are also encouraged to attend weekly events and activities including, seminars, workshops and poster sessions.

Moving On

Ralf Deitering

Ralf Deitering of the Computational Mathematics Group has accepted a new position as the Group Leader in Fluid Systems Group with the German Aerospace Center in Goettingen, Germany (<http://www.dlr.de/as/en>), effective July 1, 2013. The group is responsible for "Systems Optimization," which will include techniques for automatic shape optimization of fluid flow problems, simulate flows around high speed trains, simulation of thermal flows in plane and train cabins. The group interacts with industry partners such as Airbus and Bombardier.

Community Service

- Richard Archibald and Clayton Webster, editors, International Journal for Computer Mathematics, Special Issue on Uncertainty Quantification for High-Performance Computing
- Moet Ashfaq, visiting scientist, Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy, Visiting Scientist for Developing Countries (2012-2014)
- David E. Bernholdt reviewed for the Oak Ridge Leadership Computing Facility Director's Discretion program.
- Christian Engelmann, reviewer for Journal of Computer and System Sciences (JCSS)
- Christian Engelmann, reviewer for IEEE Transactions on Computers (TC)
- Christian Engelmann, reviewer for IEEE Transactions on Parallel and Distributed Systems (TPDS)
- Christian Engelmann, program committee for International Workshop on Runtime and Operating Systems for Supercomputers (ROSS) 2013
- Christian Engelmann, program committee for IEEE International Symposium on Parallel and Distributed Processing and Applications (ISPA)
- Christian Engelmann, program committee for International Conference on Availability, Reliability and Security (ARES) 2013
- Christian Engelmann, program committee for European MPI Users' Group Meeting (EuroMPI) 2013
- Christian Engelmann, program chair, Workshop on Resiliency in High-Performance Computing (Resilience) 2013
- X. Feng, O. Karakashian and Y. Xing, editors, Recent Developments in Discontinuous Galerkin Finite Element Methods for Partial Differential Equations, The IMA Volumes in Mathematics and its Applications, volume 157, Springer-Verlag, 2013
- Seyong Lee, program committee, ICPP, 2013
- Seyong Lee, paper review for SC, 2013
- Dong Li, program committee, EuroMPI, 2013
- Dong Li, program committee, IEEE International Conference on Big Data
- Dong Li, program committee, International Workshop on Data Intensive Computing in the Clouds (DataCloud), 2013
- Dong Li, external review for SC'13.
- Salil Mahajan, convener, Impact of Tropospheric Aerosols on Global and Regional Climate, American Geophysical Union 2013 Meeting of the Americas, Cancun, Mexico, May 2013
- Philip Roth, technical papers committee, SC13
- Philip Roth, program committee, Fourth International Workshop on Parallel Software Tools and Tool Infrastructures (PSTI 2013)
- M. Stoyanov and G. Zhang, symposium organizers, SIAM Annual 2013: Recent Advances in Numerical Methods for Partial Differential Equations with Random Inputs
- Jeffrey Vetter, program committee, HPEC, 2013
- Jeffrey Vetter, program committee, SC13 Gordon Bell Committee
- Jeffrey Vetter, program committee, Panels Committee
- Jeffrey Vetter, program committee, Emerging Technologies Committee
- Jeffrey Vetter, program committee, IEEE HiPC, 2013
- Stephen Wood - presentation, facilitation and judging of a wind turbine contest, TN-SCORE and Tennessee STEM Leadership Academy June 25-27, 2013. 70+ middle school and high school teachers from around the state participated in the conference. TN-SCORE facilitated two engineering challenges, the wind turbine competition and a microbial fuel cell competition.
- Patrick Worley, technical papers committee, SC13
- Patrick Worley (still associate editor of Parallel Computing journal)

Fourth Workshop on Data Mining in Earth System Science

June 5–7

CSMD researcher Forrest Hoffman organized the Fourth Workshop on Data Mining in Earth System Science (DMESS 2013; <http://www.climatemodeling.org/workshops/dmess2013/>) with co-conveners Jitendra Kumar (ORNL), J. Walter Larson (Australian National University, AUSTRALIA), and Miguel D. Mahecha (Max Planck Institute for Biogeochemistry, GERMANY). This workshop was held in conjunction with the 2013 International Conference on Computational Sciences (ICCS 2013; <http://www.iccs-meeting.org/iccs2013/>) in Barcelona, Spain, on June 5–7, 2013, and was chaired by J. Walter Larson. Richard T. Mills and Brian Smith of ORNL both presented papers in the DMESS 2013 session. These papers were published in volume 18 of Procedia Computer Science and are available at <http://dx.doi.org/10.1016/j.procs.2013.05.411> and <http://dx.doi.org/10.1016/j.procs.2013.05.408>

Community Service (continued)

Special Symposium on Phenology

April 14–18

CSMD researcher Forrest Hoffman co-organized a Special Symposium on Phenology with Bill Hargrove and Steve Norman (USDA Forest Service) and Joe Spruce (NASA Stennis Space Center) at the 2013 U.S.-International Association for Landscape Ecology Annual Symposium (US-IALE 2013; <http://www.usiale.org/austin2013/>), which was held April 14–18, 2013, in Austin, Texas. Hoffman also gave an oral presentation in this symposium. Titled "Developing Phenoregion Maps Using Remotely Sensed Imagery", this presentation described application of a data mining algorithm to the entire record of MODIS satellite NDVI for the conterminous U.S. at 250 m resolution to delineate annual maps of phenological regions. In addition, I was co-author on four other oral presentations at the US-IALE Symposium, including one by Jitendra Kumar (ORNL) that described an imputation technique for estimating tree suitability from sparse measurements.

6th Workshop on Resiliency in High Performance Computing (Resilience)

August 26–30

Stephen L. Scott (ORNL/TN Tech) and Christian Engelmann (ORNL) are organizing the 6th Workshop on Resiliency in High Performance Computing (Resilience) in Clusters, Clouds, and Grids in conjunction with the 19th International European Conference on Parallel and Distributed Computing (Euro-Par 2013) in Aachen, Germany, August 26-30, 2013. The Resilience workshop is a forum for researchers to present their latest advancements in the area of HPC resilience, including system-level resilience, algorithm-based fault tolerance, cross-layer resilience approaches, modeling and simulation of faults and corresponding mitigation techniques, and fault monitoring and statistical analysis. The workshop program includes presentations of peer-reviewed papers, as well as, a discussion with participants from laboratories, academia, and industry.

URL: <http://xcr.cenit.latech.edu/resilience2013>

Awards and Recognition

CSMD Researchers win two R&D 100 Awards



CSMD researchers have received two [R&D 100 awards](#), presented each year by R&D Magazine in recognition of the year's most significant technological innovations. CSMD's two bring the Lab's total of R&D 100 awards for this year to six and to 179 since their inception in 1963.

V-shaped External Cavity Laser Diode Array, was developed by ORNL's Bo Liu, Yun Liu and Yehuda Braiman. By using a V-shaped external Talbot cavity and strategically placed micro-prism mirrors, ORNL researchers have created an efficient method to extract a high-quality laser beam from a broad-area laser array, resulting in a laser source with high brightness and wavelength tunability that has applications in spectroscopy, laser radar, material surface processing and optical communications,

sensing and metrology.

Adaptable I/O System for Big Data, or ADIOS, was developed by ORNL, Georgia Institute of Technology, Rutgers University, and North Carolina State University. The ORNL team consists of Scott Klasky, Qing Liu, Norbert Podhorszki, Hasan Abbasi, Jeremy Logan, Roselyne Tchoua, Jong Youl Choi and Yuan Tian. ADIOS significantly reduces the input or output complexities encountered by scientists running on high performance computers, along with reducing their time to solution, which allows researchers to spend more time achieving scientific insight and less time managing data.

Oscar Hernandez Named Director

The OpenACC standards organization has named CSMD researcher Oscar Hernandez as Director of Developer Adoption. This appointment recognizes Oscar's energetic work bringing user input to the development of the standard, and evangelizing OpenACC as a portable approach to the programming of accelerators. Hernandez has served as representative to the standards body since ORNL became the first non-vendor user-oriented organization to join in January 2013.

Chuck Glover (Certificate of Appreciation)

Chuck Glover was awarded a Certificate of Appreciation by the Missile Defense Agency. Chuck's certificate reads that he "is to be commended for his outstanding support to the Command and Control, Battle Management, and Communications (C2BMC) Program Office during Austere Challenge 2012 (AC-12) Exercise. AC-12 is a high visibility exercise sponsored by the Chairman of the Joints Chiefs of Staff and resourced by U.S. European Command and is held in conjunction with Host Nation missile and defense forces. His dedication in expediting contract actions, infrastructure upgrades, equipment modifications for data

Awards and Recognition (continued)

collection, event planning, execution, and data analysis led to the overall success of AC-12. Mr Glover is an outstanding contributor to our mission success and his efforts reflect credit upon himself, the C2BMC Program Office, and the Missile Defense Agency."

Pratul Agarwal (Patent)

Pratul Agarwal was awarded U.S. Patent No. 8,417,461 for "Identification and Modification of Dynamical Regions in Proteins for Alteration of Enzyme Catalytic Effect"

According to the patent's abstract, the patent covers "A method for analysis, control, and manipulation for improvement of the chemical reaction rate of a protein-mediated reaction is provided. Enzymes, which typically comprise protein molecules, are very efficient catalysts that enhance chemical reaction rates by many orders of magnitude. Enzymes are widely used for a number of functions in chemical, biochemical, pharmaceutical, and other purposes. The method identifies key protein vibration modes that control the chemical reaction rate of the protein-mediated reaction, providing identification of the factors that enable the enzymes to achieve the high rate of reaction enhancement. By controlling these factors, the function of enzymes may be modulated, i.e., the activity can either be increased for faster enzyme reaction or it can be decreased when a slower enzyme is desired. This method provides an inexpensive and efficient solution by utilizing computer simulations, in combination with available experimental data, to build suitable models and investigate the enzyme activity."

Jack Dongarra (Professional Achievement Award)

Jack Dongarra, CSMD Researcher, Distinguished Professor in the Department of Electrical Engineering and Computer Science at UTK and the director of the Innovative Computer Laboratory, will be the recipient of the 2013 Illinois Institute of Technology's (IIT) Professional Achievement Award in recognition of the contribution and achievements of IIT's most remarkable graduates and leaders. Dongarra received his MS degree from IIT. The awards ceremony will take place on the IIT campus in April.

Researchers Win Gauss Award

Three ORNL researchers were a part of the team that received international recognition. The team was given the Gauss Award at the International Supercomputing Conference (ISC) for the most outstanding paper in the field of scalable supercomputing.

The paper, "TUE, a New Energy-Efficiency Metric Applied at ORNL's Jaguar," outlines how to get a more accurate representation of the data-center energy efficiency. Two new metrics are proposed; they are ITUE (IT-power Usage Effectiveness) and TUE (Total-power Usage Effectiveness). Currently, Power Usage Effectiveness (PUE) is used to measure the efficiency. ITUE is similar to PUE but "inside" the IT. TUE combines the two for a total efficiency picture. It provides a ratio of total energy, separating internal and external support energy uses from the specific energy used in the HPC. The paper concludes with a field application of the method at ORNL's Jaguar supercomputer.

The research was a collaboration between government, national labs and industry aimed at being better able to ensure the most accurate and wise use of power going forward for computer systems and computing facilities. The team includes Chung-Hsing Hsu, Stephen W. Poole and Don E. Maxwell, ORNL; Michael K. Patterson, Intel; William Tschudi and Henry Coles, LBNL; David J. Martinez, SNL; and Natalie Bates, Energy Efficient HPC Working Group (EEHPC WG).

At ORNL, power-aware computing has been an active area of research, also a focal point, within the DoD funded program within Computer Science and Mathematics Division. We have done a fairly large body of this work, and Dr. Chung-Hsing worked in this area when he was at Los Alamos National Laboratory.

Going forward, the team plan to measure energy efficiency at other facilities to further develop TUE. The ISC organizers have requested that the researchers return for ISC 2014 to follow up on the work after TUE is measured at more supercomputing facilities. ORNL will continue down this research path and develop it as much as possible. We are currently working with the EEHPC WG to create guidelines for procurement documents that include energy considerations.

"Over time, TUE and ITUE can create the same pull and success that PUE has and further improve the energy efficiency of supercomputers and computing facilities," says Dr. Hsu.

The Gauss Award is sponsored by the German Gauss Center for Supercomputing, a collaboration of the German national supercomputing centers at Garching, Jülich and Stuttgart, and is presented annually at ISC. ISC is the oldest global conference and exhibition for high performance computing and drew 2,500 attendees this year. A committee chooses the most outstanding paper in the field of scalable supercomputing from all of the papers submitted for Research Paper Sessions. The winner of the award receives a 3,000 Euro prize and presents their paper at the conference.

Events

Seminars

- June 28, 2013 - Yuri Melnikov: [A surprising connection between Green's functions and the infinite product representation of elementary functions](#)
- June 27, 2013 - Kimmy Mu: [Performance, accuracy and power tradeoff for scientific processes using workflow in high performance computing](#)
- June 26, 2013 - Matthew Causley: [A fast implicit Maxwell field solver for plasma simulations](#)
- June 25, 2013 - Jeff Haack: [Conservative Spectral Method for Solving the Boltzmann Equation](#)
- June 17, 2013 - Megan Cason: [Analytic Utility Of Novel Threading Models In Distributed Graph Algorithms](#)
- June 14, 2013 - Jeff Carver: [Applying Software Engineering Principles to Computational Science](#)
- June 12, 2013 - Hans-Werner van Wyk: [Multilevel Quadrature Methods](#)
- June 7, 2013 - Xuechen Zhang: [Scibox: Cloud Facility for Sharing On-Line Data](#)
- June 6, 2013 - Yuan Tian: [Taming Scientific Big Data with Flexible Organizations for Exascale Computing](#)
- May 31, 2013 - Pablo Seleson: [Multiscale Material Modeling with Peridynamics](#)
- May 29, 2013 - Ryan McMahan: [The Effects of System Fidelity for Virtual Reality Applications](#)
- May 28, 2013 - Adrian Sandu: [Data Assimilation and the Adaptive Solution of Inverse Problems](#)
- May 24, 2013 - Satoshi Matsuoka: [The Futures of Tsubame Supercomputer and the Japanese HPCI Towards Exascale](#)
- May 17, 2013 - Jon Mietling and Tony McCrary: [Bling3D: a new game development toolset from I33t Labs](#)
- May 10, 2013 - Xiao Chen: [A Modular Uncertainty Quantification Framework for Multi-physics Systems](#)
- May 2, 2013 - Kenley Pelzer: [Quantum Biology: Elucidating Design Principles from Photosynthesis](#)
- April 23, 2013 - Kirk W. Cameron: [Power-Performance Modeling, Analyses and Challenges](#)
- April 23, 2013 - Jordan Deyton: [Tor Bridge Distribution Powered by Threshold RSA](#)
- April 19, 2013 - Maria Avramova and Kostadin Ivanov: [OECD LWR UAM and PSBT/BFBT benchmarks and their relation to Advanced LWR Simulations](#)
- April 18, 2013 - Sparsh Mittal: [MASTER: A Technique for Improving Energy Efficiency of Caches in Multicore Processors](#)
- April 17, 2013 - Okwan Kwon: [Automatic Scaling of OpenMP Applications Beyond Shared Memory](#)
- April 17, 2013 - Michael S. Murillo: [Molecular Dynamics Simulations of Charged Particle Transport in High Energy-Density Matter](#)
- April 12, 2013 - Vivek K. Pallipuram: [Exploring Multiple Levels Of Performance Modeling For Heterogeneous Systems](#)
- April 11, 2013 - Jeff Young: [Commodity Global Address Spaces - How Can We Scale Out Accelerator and Memory Performance for Tomorrow's Clusters?](#)
- April 9, 2013 - Cong Liu: [Towards Efficient Real-Time Multicore Computing Systems](#)
- April 9, 2013 - Frank Mueller: [On Determining a Viable Path to Resilience at Exascale](#)
- April 5, 2013 - Sarat Sreepathi: [Optimus: A Parallel Metaheuristic Optimization Framework With Environmental Engineering Applications](#)

Upcoming Events

OpenSHMEM Workshop

Annapolis, Maryland
October 23–25

The OpenSHMEM workshop is an annual event dedicated to the promotion and advancement of parallel programming with the OpenSHMEM programming interface and its future direction. It is the premier venue to discuss and present the latest developments, implementation technology, trends, recent research ideas and results related to OpenSHMEM and its use in applications. This year's workshop will also emphasize accelerator APIs (e.g. OpenACC or OpenCL) and their use in conjunction with OpenSHMEM.. The workshop is organized as a two day event. The first day will consists of talks and tutorials on OpenSHMEM and related technologies and extensions such as OpenSHMEM I/O, UCCS and Compilers, Performance and debugging tools (such as the OpenSHMEM Analyzer, TAU , VampirTrace, DDT). The second day will focus on the latest developments with respect to the OpenACC API for accelerators and the use of OpenACC with OpenSHMEM. At the end of the workshop we will have a panel session to discuss the future direction of OpenSHMEM and to solicit feedback from the community on what should be included in the next major OpenSHMEM specification.

Please visit <http://www.csm.ornl.gov/workshops/openshmem2013/> for more information.

Publications/Presentations

Abstract - Conference

- Mahajan, Salil (ORNL), Evans, Katherine J. (ORNL), Hack, James J. (ORNL), Truesdale, John (National Center for Atmospheric Research (NCAR)). Linearity of Climate Response to Increases in Black Carbon Aerosols, AGU Meeting of the Americas 2013, Cancun, May 2013
- Fann, George I. (ORNL). Adaptive Pseudo-Spectral Method for Solving HFB Equations, International Conference on Nuclear Theory in the Supercomputing Era - 2013, Ames, 2013
- Liu, Bo (ORNL), Braiman, Yehuda (ORNL). Near Diffraction Limit Coherent Addition of Broad-Area Laser Diode Array, Directed energy professional society, Advanced High-Power Lasers, Santa Fe, June 2013
- Radhakrishnan, Balasubramaniam (ORNL), Gorti, Sarma B. (ORNL), Clarno, Kevin T. (ORNL), Yan, Yong (ORNL). Phase Field Simulations of Hydride Reorientation in Zircalloys, International High-Level Radioactive Waste Management Conference, Albuquerque, April 2013
- Ashfaq, Moetasim (ORNL), Touma, Danielle E. (ORNL), Nayak, Munir A. (ORNL), Kao, Shih-Chieh (ORNL). Changes in drought characteristics in the 21st century, American Geophysical Union Fall Meeting 2012, San Francisco, 2012

Abstract - No Conference

- Fann, George I. (ORNL). MADNESS: a scalable and adaptive approach for solving integro-differential equations in 3+D, 2013
- Philip, Bobby (ORNL). 3D Structured Adaptive Mesh Refinement and Multilevel Preconditioning for Non-Equilibrium Radiation Diffusion, April 2013
- Philip, Bobby (ORNL). The Advanced Multi-Physics Framework With An Application to Nuclear Fuel Simulations, April 2013

Book Chapter - Article

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Journal Article

- Barton, Philip T. (California Institute of Technology, Pasadena), Deiterding, Ralf (ORNL), Meiron, Daniel I. (California Institute of Technology, Pasadena), Pullin, Dale I (California Institute of Technology, Pasadena). Eulerian adaptive finite-difference method for high-velocity impact and penetration problems Journal of Computational Physics, May 2013
- Deiterding, Ralf (ORNL), Glowinski, R. (University of Houston, Houston), Oliver, Hilde (ORNL), Poole, Stephen W. (ORNL). A Reliable Split-Step Fourier Method for the Propagation Equation of Ultra-Fast Pulses in Single-Mode Optical Fibers Journal of Lightwave Technology, June 2013
- Fann, George I. (ORNL). Computational nuclear quantum many-body problem: The UNEDF project Computer Physics Communications, June 2013

Publications/Presentations (continued)

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ORNL Report

- Lothian, Josh (ORNL), Baker, Matthew B. (ORNL), Schrock, Jonathan (ORNL), Poole, Stephen W. (ORNL), Kuehn, Jeffery A. (ORNL). SystemBurn: Principles of Design and Operation Release 3.1, June 2013

Other

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- Radhakrishnan, Balasubramaniam (ORNL), Gorti, Sarma B. (ORNL), Yan, Yong (ORNL), Clarno, Kevin T. (ORNL). Phase Field Simulations of Hydride Reorientation in Zircalloys, 2013 International High-Level Radioactive Waste Management Conference, Albuquerque, April 2013

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- Ashfaq, M., Near-term acceleration of hydroclimatic change in the western U.S, European Geophysical Union 2013, Apr 7-12, 2013, Vienna, Austria.
- Ashfaq, M., South Asia: A case for high-resolution climate modeling, European Geophysical Union 2013, Apr 7-12, 2013, Vienna, Austria.
- Berry, Donald K., Joseph Schuchart, and Robert Henschel, Experiences Porting a Molecular Dynamics Code to GPUs on a Cray XK7, Proceedings of the Cray User Group 2013, Nappa Valley, CA.
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- Mahajan S., K. J. Evans, J. J. Hack and J. E. Truesdale (2013): Linearity of climate response to increases in black carbon aerosols, *Journal of Climate* (accepted)
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- Marin, G., McCurdy, C., and Vetter, J.S., "Diagnosis and Optimization of Application Prefetching Performance," in ACM International Conference on Supercomputing (ICS). Portland: ACM, 2013
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- Patterson, M.K. Poole, S.W. Hsu, C. Maxwell, D. Tschudi, W. Coles, H. Martinez D.J. and Bates N. "TUE, A New Energy-Efficiency Metric Applied at ORNL's Jaguar." International Supercomputing Conference, June 2013.
- Philip, Bobby (ORNL). 3D Structured Adaptive Mesh Refinement and Multilevel Preconditioning for Non-Equilibrium Radiation Diffusion
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- Pokhriyal, N. U. Mertuyrek, A. Godfrey, J. J. Billings "Knowledge Discovery from Nuclear Reactor Simulation Data", at the International Workshop on Analytics for Cyber-physical Systems, which was held in conjunction with SIAM Data Mining 2013 on May 4th Austin, TX.
- Radhakrishnan, Balasubramaniam (ORNL), Gorti, Sarma B. (ORNL), Clarno, Kevin T. (ORNL), Yan, Yong (ORNL). Phase Field Simulations of Hydride Reorientation in Zircalloys, International High Level Radioactive Waste Management Conference, Albuquerque
- Rao N. S. V., First Conference on Validating Models of Adversary Behaviors, June 23-26, 2013, Niagara Falls, NY.
- Rao N. S. V., Department of Computer Science, April 12, 2013, Florida International University, Miami, FL.
- Rao N. S. V., Poole S. W., Ma C. Y. T., He F., Zhuang J., Yau D. K. Y., Infrastructure resilience using cyber-physical game-theoretic approach, International Symposium on Resilient Cyber System, Resilience Week, 2013.
- Rao N. S. V., Chaotic maps for robustness estimation of Exascale computations DOE Applied Mathematics PI Meeting, abstract, 2013.
- Rao N. S. V., Poole S. W., Ma C. Y. T., He F., Zhuang J., Yau D. K. Y., Cyber and physical information fusion for infrastructure protection: A game-theoretic approach, International Conference on Information Fusion, July 9-12, 2013, Istanbul, Turkey.
- Rao N. S. V., Poole S. W., Ma C. Y. T., He F., Zhuang J., Yau D. K. Y., Game-Theoretic approach to cyber-physical infrastructures: Discrete models and UltraScience Net case study, abstract, First Conference on Validating Models of Adversary Behaviors, June 23-26, 2013, Niagara Falls, NY.
- Rao N. S. V., Fault detection in multi-core processors using chaotic maps, 3rd Workshop on Fault- Tolerance for HPC at Extreme Scale (FTXS 2013), June 18, 2013, New York, NY.
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- Reuter, Matthew G. (ORNL), Williams, Patrick D. (ORNL). The Information Content of Conductance Histogram Peaks: Transport Mechanisms, Level Alignments, and Coupling Strengths, 2013 March Meeting of the American Physical Society, Baltimore
- Roth, P.C., "Tracking a Value's Influence on Later Computation," accepted to 6th Workshop on Productivity and Performance (PROPER 2013), Aachen, Germany, 2013.
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- Stoyanov, Miroslav K. (ORNL). Algorithm Resilience with Respect to Hardware Faults, SIAM SEAS 2013, Knoxville
- Sumpter, Bobby G. (ORNL). Nanomaterials Theory Institute and Computational Chemical and Materials Sciences
- Touma, Danielle E. (ORNL), Nayak, Munir A. (ORNL), Kao, Shih-Chieh (ORNL), Ashfaq, Moetasim (ORNL). Changes in Drought Characteristics of the 21st Century CMIP5 Climate Projection, European Geosciences Union General Assembly 2013, Vienna
- Vetter, J.S., "Automated Exploration of the HPC Codesign Space," in International HPC Forum (IHPCF). Changsha, China, 2013
- Wang, Bin., Wu, Bo., Li, Dong., Shen, Xipeng., Yu, Weikuan., Jiao, Yizheng., Vetter, Jeffrey S., "Exploring Hybrid Memory for GPU Energy Efficiency through Software-Hardware Co-Design", accepted in International Conference on Parallel Architectures and Compilation Techniques (PACT), 2013
- Webster, C. Adaptive multilevel stochastic collocation methods for accelerating solutions of PDEs with random input data, 9th International Conference on Large-Scale Scientific Computations, Sozopol, Bulgaria, Jun. 2013
- Webster, C., Adaptive multilevel stochastic collocation methods for accelerating solutions of PDEs SIAM Annual Meeting, San Diego, CA, July 2013
- Webster, C., Adaptive sparse grid stochastic collocation methods for PDEs with random input data, Colloquium talk, Department of Mathematics, Auburn University, Auburn AL, Apr. 2013
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- Zhang, G., A Hyper-spherical sparse-grid method for high-dimensional discontinuity detection 9th International Conference on Large-Scale Scientific Computations, Sozopol, Bulgaria, Jun. 2013
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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 eight Groups. These Groups and their Group Leaders are:

- Complex Systems - Jacob Barhen
- Computational Chemical and Materials Sciences - Bobby Sumpter
- Computational Earth Sciences - Kate Evans (Interim)
- Computational Engineering and Energy Sciences - John Turner
- Computational Mathematics - Barney Maccabe
- Computer Science Research – David Bernholdt
- Future Technologies - Jeff Vetter
- Scientific Data - Scott Klasky

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.



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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