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QUARTERLY NEWSLETTER FOR
THE COMPUTER SCIENCE AND
MATHEMATICS DIVISION

# CSMD

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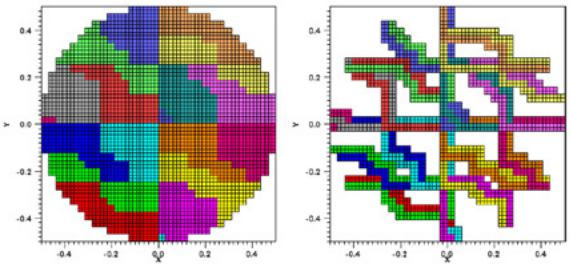
## Science Highlights

### Simulation Framework for Multi-Scale, Multi-Physics Applications

*ORNL Team Members: Christian Y. Cardall and Eirik Endeve - ORNL, with Reuben D. Budiardja - NICS and Anthony Mezzacappa - JICS/UTK*

A team comprised of researchers from ORNL, NICS, and JICS/UTK are developing a code, General Astrophysical Simulation System (GenASiS), for multi-scale, multi-physics simulations of core-collapse supernovae on leadership computing facility architectures. In their paper, GenASiS: General Astrophysical Simulation System. I. Refinable Mesh And Nonrelativistic Hydrodynamics, the team documents methods for compressible hydrodynamics on a multi-level mesh suitable for supernova simulations. The developments have laid the foundation for implementation of additional physics solvers, including solvers for gravitational field and radiation transport equations. Following object-oriented principles, GenASiS is designed to refer to multiple algorithms for physics solvers with abstracted names and/or interfaces. As such, it has the potential to become a valuable simulation framework for multiple application areas.

Cardall, C.Y., Budiardja, R.D., Endeve, E., & Mezzacappa, A. 2013, "GenASiS: General Astrophysical Simulation System. I. Refinable Mesh And Nonrelativistic Hydrodynamics," the Astrophysical Journal Supplement Series, in press



***Domain decomposition of a spherical submesh, illustrating proper cells (left) and the ghost cells partially bounding them (right). The ghost cells of the different processes partially overlap. Each individual cell is pictured; two dimensions, low resolution, and a small number of processes (16) are used for clarity.***

OAK RIDGE National Laboratory

# Science Highlights [Continued]

### Supporting the Development of Resilient Message Passing Applications using Simulation

*ORNL Team Members: Thomas Naughton, Christian Engelmann, Geoffroy Vallée, and Swen Böhm*

An emerging aspect of high-performance computing (HPC) hardware/software co-design is investigating performance under failure. Recent work at Oak Ridge National Laboratory extends the Extreme-scale Simulator (xSim), which was designed for evaluating the performance of Message Passing Interface (MPI) applications on future HPC architectures, with fault-tolerant MPI extensions proposed by the MPI Fault Tolerance Working Group. xSim permits running MPI applications with millions of concurrent MPI ranks, while observing application performance in a simulated extreme-scale system using a lightweight parallel discrete event simulation.

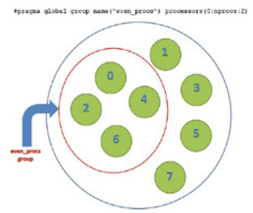
The newly added features offer user-level failure mitigation (ULFM) extensions at the simulated MPI layer to support algorithm-based fault tolerance (ABFT). The approach permits investigating performance under failure and failure handling of ABFT solutions. The newly enhanced xSim is the very first performance tool that supports ULFM and ABFT.

Thomas Naughton, Christian Engelmann, Geoffroy Vallée, and Swen Böhm. **Supporting the Development of Resilient Message Passing Applications using Simulation.** In Proceedings of the 22nd Euromicro International Conference on Parallel, Distributed, and network-based Processing (PDP) 2014, Turin, Italy, February 12-14, 2014. IEEE Computer Society, Los Alamitos, CA, USA.

### A Global View Programming Abstraction for Transitioning MPI Codes to PGAS Languages

*ORNL Team Members: Tiffany M. Mintz, Oscar Hernandez, and David E. Bernholdt*

The multicore era of computing has provided us with Peta-scale supercomputing machines with distributed shared memory architectures, known as the Non-Uniform Memory Access (NUMA) architecture, that exploit the advantages of both the data and message passing parallel paradigms. While the multicore, NUMA architecture enables fast data movement and the potential for easy programmability, the current standard for programming scientific applications for parallel execution does not truly exploit these advantages. A sufficient programming model would need to provide mechanisms for managing data locality as well as take advantage of the global view of data provided by the architecture.




*Example using group directive to create the group 'even proc'*

The partitioned global address space (PGAS) programming model is a promising approach to parallel programming with a primary focus on simplifying programming and exploiting data locality. PGAS languages like X10 and Chapel were designed to support highly productive programming for ultra-scale HPC systems and merge the concepts of global views of data, tasks and locality.

Although PGAS languages have yet to be fully adopted by the general HPC community, we are encouraged by the continued progress being made in the development of Chapel and the lessons learned from other languages like HPF, X10 and ZPL. So with a focus on aiding the adoption of PGAS languages by computational scientists in the HPC community, we have developed a set of directives based language extensions to express the global view of data in SPMD codes. The directives provide high-level descriptions of data distributions, parallel computation and inter-processor data movement, as well as high-level expressions for arranging and grouping processors. With these directives, the programmer is able to identify the regions of their application that map well to the high level constructs provided by PGAS languages, and incrementally transition their source code to these languages.

Read more **HERE**.

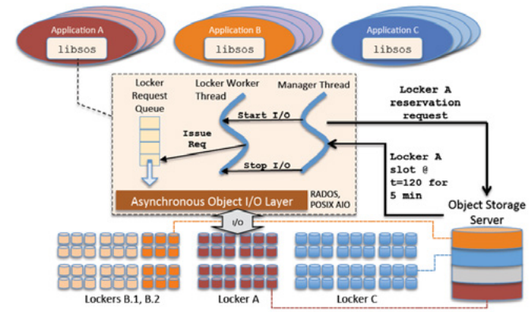
### Asynchronous Object Storage with QoS for Scientific and Commercial Big Data

*ORNL Team Members: Michael J. Brim, David A. Dillow, Sarp Oral, Bradley W. Settlemyer, Feiyi Wang*

ORNL researchers Michael J. Brim, David A. Dillow, Sarp Oral, Bradley W. Settlemyer, and Feiyi Wang presented the paper Asynchronous Object Storage with QoS for Scientific and Commercial Big Data at the 8th Parallel Data Storage Workshop (held in conjunction with



# Science Highlights [Continued]




*Scalable Object Storage Architecture*

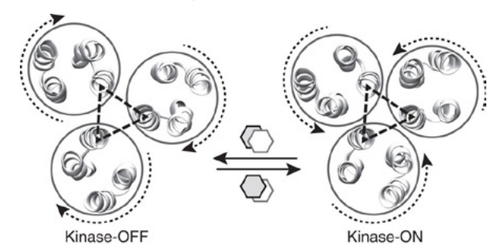
This paper presents the team's design for an asynchronous object storage system intended for use in scientific and commercial big data workloads. Use cases from the target workload domains are used to motivate the key abstractions used in the application programming interface (API). The architecture of the Scalable Object Store (SOS), a prototype object storage system that supports the API's facilities, is presented. The SOS serves as a vehicle for future research into scalable and resilient big data object storage. Experimental results showing storage device interference from competing workloads are used to motivate the team's initial research in providing quality of service (QoS) contracts to SOS clients.

Read more **HERE**.

### A phenylalanine rotameric switch for signal-state control in bacterial chemoreceptors

*Davi R. Ortega, Chen Yang, Peter Ames, Jerome Baudry, John S. Parkinson, and Igor B. Zhulin*

Bacterial chemoreceptors are widely used as a model system for elucidating the molecular mechanisms of transmembrane signalling and have provided a detailed understanding of how ligand binding by the receptor modulates the activity of its associated kinase CheA.




*Model for modulation of kinase activity by receptor trimers of dimers.*

However, the mechanisms by which conformational signals move between signalling elements within a receptor dimer and how they control kinase activity remain unknown. Here, using long molecular dynamics simulations, we show that the kinase-activating cytoplasmic tip of the chemoreceptor fluctuates between two stable conformations in a signal-dependent manner. A highly conserved residue, Phe396, appears to serve as the conformational switch, because flipping of the stacked aromatic rings of an interacting F396-F396' pair in the receptor homodimer takes place concomitantly with the signal-related conformational changes. We suggest that interacting aromatic residues, which are common stabilizers of protein tertiary structure, might serve as rotameric molecular switches in other biological processes as well.

Nature Communications 4, Article number: 2881
doi:10.1038/ncomms3881
Received 15 August 2013 | Accepted 07 November 2013 | Published 13 December 2013
**http://www.nature.com/ncomms/2013/131213/ncomms3881/full/ncomms3881.html**

### Oak Ridge National Laboratory Researchers Improve Fidelity of Earth System Models

*Forrest Hoffman*

Oak Ridge National Laboratory (ORNL) researchers are partnering with other Department of Energy (DOE) laboratories to improve the supercomputing applications that deliver breakthroughs in climate science.

Forrest Hoffman, Kate Evans, James Hack, and other scientists at ORNL's Climate Change Science Institute participate in three projects funded through the Scientific Discovery through Advanced Computing, or SciDAC, Program. These projects aim to improve the Community Earth System Model, a megamodel that couples interactive component models of the atmosphere, ocean, land, and sea and land ice. ORNL scientists are integrating multiscale algorithms to better simulate atmospheric and oceanic phenomena, verifying the accuracy of ice sheet simulations, and improving the representation of biogeochemical cycles on land and in the ocean and atmosphere. These researchers and dozens of others run Earth system models on the Oak Ridge Leadership Computing Facility's Titan supercomputer.

"These projects are designed to advance the simulation and predictive capabilities of the models," said Hoffman, one of the SciDAC principal investigators. "These projects partner climate scientists, mathematicians, and computer scientists to improve the accuracy and scientific fidelity of these complex models and to deliver a new generation of Earth system models with unsurpassed performance on the leadership class computing facilities that DOE operates."

- by *Jennifer Brouner*

Link - **http://climatechangescience.ornl.gov/content/oak-ridge-national-laboratory-researchers-improve-fidelity-earth-system-models**

### A Runtime Environment for Supporting Research in Resilient HPC System Software & Tools

*ORNL Team Members: Geoffroy Vallee, Thomas Naughton, Swen Boehm, and Christian Engelmann*

The high-performance computing (HPC) community continues to increase the size and complexity of hardware platforms that support advanced scientific workloads. The runtime environment (RTE) is a crucial layer in the software stack for these large-scale systems. The RTE manages the interface between the operating system and the application running in parallel on the machine. The deployment of applications and tools on large-scale HPC computing systems requires the RTE to manage process creation in a scalable manner, support sparse connectivity, and provide fault tolerance. We have developed a new RTE that provides a basis for building distributed execution environments and developing tools for HPC to aid research in system software and resilience. This paper describes the software architecture of the Scalable runTime Component Infrastructure (STCI), which is intended to provide a complete infrastructure for scalable start-up and management of many processes in large-scale HPC systems. We highlight features of the current implementation, which is provided as a system library that allows developers to easily use and integrate STCI in their tools and/or applications. The motivation for this work has been to support ongoing research activities in fault-tolerance for large-scale systems. We discuss the advantages of the modular framework employed and describe two use cases that demonstrate its capabilities: (i) an alternate runtime for a Message Passing Interface (MPI) stack, and (ii) a distributed control and communication substrate for a fault-injection tool.

Geoffroy Vallée, Thomas Naughton, Swen Böhm, and Christian Engelmann. "A Runtime Environment for Supporting Research in Resilient HPC System Software & Tools." In Proceedings of the 1st International Symposium on Computing and Networking – Across Practical Development and Theoretical Research – (CANDAR) 2013, Matsuyama, Japan, December 4-6, 2013. IEEE Computer Society, Los Alamitos, CA, USA. To appear.

Read more **HERE** and **HERE**.

### Titan Early Science - High-Fidelity Neutronic Analysis of the Westinghouse AP1000

*Principle Investigators:*
*ORNL: John Turner (ORNL/CSMD), Tom Evans (ORNL/RNSD), Andrew Godfrey (ORNL/RNSD); Westinghouse Nuclear: Fausto Franceschini; Co-Investigators (alphabetical): Wayne Joubert (ORNL/NCCS) and Steven Hamilton (ORNL/RNSD)*

As part of the OLCF Early Science program, a proposal to simulate Westinghouse AP1000 startup using three neutronics approaches implemented within the VERA neutronics package, Exnihilo, was granted an allocation of 60 million core-hours.

The three neutronics approaches to be applied to the AP1000 are:

- a low-order SP_N method of 3D deterministic neutron transport with pin-homogenized cross sections, which typically requires ~1000 compute cores,
- Denovo, a higher-order S_N method of 3D deterministic neutron transport using the KBA parallel algorithm, with excellent scaling up to the entire Titan system, including GPUs,
- Shift, a new high-fidelity continuous energy Monte Carlo based transport code that can also scale up to the entire Titan system and which will provide a reference solution for reactivity and nuclear fission rate distribution due to its rigorous spatial and energy treatment.

Denovo, the deterministic neutron transport capability that has been under development at ORNL over the last several years, has been accelerated via CUDA implementation of the underlying wavefront algorithm as part of the Center for Accelerated Application Readiness (CAAR).





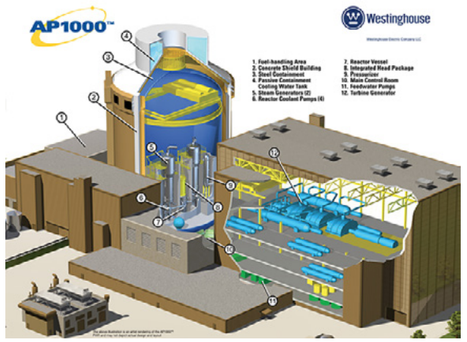



*Image: Westinghouse*

The Shift Monte Carlo results will rival, and potentially exceed, previous simulations, with respect to both fidelity (1 trillion particles or more) and geometry (a full reactor core), and these results have the potential to provide reference benchmark solutions to the reactor analysis community for years to come. Although Shift has not yet been modified to take advantage of GPU acceleration, that effort is planned, and these results will also serve to provide performance data and inform that work.

Together, these neutronics capabilities provide a range of approaches that trade fidelity and computational resource requirements. Choosing the most appropriate approach requires an understanding of these tradeoffs, and Exnihilo provides a unique ability to characterize these methods more directly than ever before, at unprecedented scales, on problems of immediate relevance for the nuclear industry.

Read more **HERE**.

### End-to-End Data Movement Using MPI-IO Over Routed Terabits Infrastructures

*ORNL Team Members: Geoffroy Vallee, Scott Atchley, Youngjae Kim, and Galen Shipman*

Scientific discovery is nowadays driven by large-scale simulations running on massively parallel high-performance computing (HPC) systems. These applications each generate a large of data, which then needs to be post-processed for example for data mining or visualization. Unfortunately, the computing platform used for post processing might be different from the one on which the data is initially generated, introducing the challenge of moving large amount of data between computing platforms. This is especially challenging when these two platforms are geographically separated since the data needs to be moved between computing facilities. This is even more critical when scientists tightly couple their domain specific applications with a post processing application.

The paper presents a high-throughput end-to-end data movement solution for parallel applications that is based on parallel access to data files and the Message Passing Interface (MPI) over the Common Communication Infrastructure (CCI). To demonstrate the benefit of the proposed solution, we present experiments for data transfer between MPI applications over a dedicated terabit routed infrastructure, using the Energy Sciences Network (ESnet) that connects the U.S. Department of Energy (DOE) national laboratories.

Geoffroy Vallee, Scott Atchley, Youngjae Kim, and Galen Shipman. End-to-End Data Movement Using MPI-IO Over Routed Terabits Infrastructures. In Proceedings of the 3rd IEEE/ACM International Workshop on Network-aware Data Management (NDM 2013), held in conjunction with SuperComputing 2013. Denver, CO, USA. November 17, 2013

Read more **HERE** and **HERE**.

### Computational Infrastructure for Nuclear Astrophysics (CINA) 2.1

The Computational Infrastructure for Nuclear Astrophysics (CINA) is a cloud computing system that enables users the capability to robustly simulate, share, store, analyze and visualize explosive nucleosynthesis events such as novae, X-ray bursts and core-collapse supernovae via a web-deliverable, easy-to-use, Java application. Users can also upload, modify, merge, store and share the complex input data required by these simulations. Version 2.1 expand CINA's set of simulation types to include the cold rapid neutron process (cold r-process), which takes place in the supernovae environment. This release also allows users to generate 1D plots comparing simulation results to over a dozen observational datasets and 1D plots displaying the fractional difference between simulation results and the available observations. The plotted data can then be downloaded in tabular form. In addition, version 2.1 enhances the Element Synthesis Animator tool by allowing users to restrict the proton number range of results plotted on the animated chart of the nuclides. This capability allows users to zoom in on a particular region of the nuclide chart and export images and movies of the selected region of interest.

Contact: Eric Lingerfelt, lingerfeltej@ornl.gov
URL: **www.nucastrodata.org/infrastructure**

# Software

### National Isotope Development Center (NIDC) Online Management Toolkit Online Management Toolkit (OMT) 1.2

The National Isotope Development Center (NIDC) Online Management Toolkit (OMT) provides NIDC staff the capability to quickly and securely modify the product catalog, harvest website statistics, dynamically generate monthly reports, and administer OMT user accounts with a web-deliverable, cross-platform Java application. A major milestone in the Isotope Business Office Business Systems Upgrade (IBOBSU) project has been achieved with the release of OMT 1.2. A central goal of IBOBSU is to create a NIDC Preferred Customer Portal at isotopes.gov that allows vetted research customers the ability to create quotes and submit orders for stable isotopes in inventory via the website. The latest OMT tool, called the "Preferred Customer Manager", allows NIDC staff to explore, activate, deactivate and reactivate Preferred Customer accounts. It also allows staff to modify these accounts and information concerning the institution each customer represents.

Contact: Eric Lingerfelt, lingerfeltej@ornl.gov
URL: **http://isotopes.gov**

### ADIOS 1.6 Update Released

The main novelty in this release was the introduction of data transformations. Any data transformation that can be executed concurrently on each processor without communication now can be implemented as a specific transform method in ADIOS, and applied to the output data on a per-variable basis. In this release, lossless compression methods, like zlib, szip, bzip2 methods and ISOBAR developed by NCSU, were included. There is on—going work on adding lossy compression and data indexing methods. Another extension to ADIOS was the new functions in the Read API to get information about the visualization schema embedded in the ADIOS output data. These functions, developed by Kimmy Mu, simplify and standardize the processing of schema information. The upcoming release of VisIt (version 2.8) will include the generic ADIOS reader that will support any application that produces data with schema using ADIOS. While the file writing performance of ADIOS was always outstanding on OLCF resources, Bluegene/Q has a specific I/O infrastructure that can provide higher and more scalable performance then what current ADIOS methods can utilize. Gary Liu has developed a new, BG/Q specific, topology-aware aggregation method that optimizes the routing of data from the compute nodes to the I/O nodes. This new method has already achieved 128GB/sec write 1performance for an INCITE application on the quarter size of Mira at ALCF. Smaller improvements in this release include the speedup in metadata handling in the memory, which eliminates performance problems experienced by some applications writing tens of thousands of variables into a single file. Moreover, the ADIOS automake build is more flexible now, separating the build from the source.

### NiCE 2.1.3 adds support for sodium-cooled fast reactors, enhanced usability

*Contact: Jay Jay Billings <billingsjj@ornl.gov>*
*Co-authors: Jordan Deyton, Taylor Patterson, Anna Wojtowicz*

Version 2.1.3 of the NEAMS Integrated Computational Environment (NiCE) was released on December 13th 2013. New plugins were developed in NiCE to create input files and add job launch capabilities for Argonne National Laboratory's Simulation-based High efficiency Advanced Reactor Prototyping (SHARP) simulator for SFRs, which was also installed on ORNL machines for the first time as part of this release. Input file generation for SHARP covers all of the current neutronics parameters support by the input specification and a future release will include support for fluid dynamics and structural mechanics. NiCE's Reactor Analyzer - a tool for investigating simulation results for nuclear reactors in an intuitive, domain-specific way - was extended and now includes support for SFRs in addition to its support of Light-Water Reactors (LWRs) from a previous release. This included the development of new hex and elliptical grids in the user interface to view the unique geometry of SFR components and a detailed model in the Unified Modeling Language (UML) of a conceptual SFR. This release also included several usability enhancements since one of the most significant challenges for a modeling and simulation environment is exposing information to users in a way that gives them everything they need and no more without overloading them. NiCE 2.1.3 is the first release of NiCE to include support for both the Fuels and Reactors Product Lines of the Nuclear Energy Advanced Modeling and Simulation (NEAMS) and is also the first NEAMS product to be funded by the ARC program as part of a technology transfer exercise to deploy NEAMS products to users ahead of schedule.

In addition to software enhancements, we have released six YouTube videos covering our new plugins for the CAEBAT and MOOSE packages as well as the "rebuilt" Reactor Analyzer. These videos were well received by the usual audience, but they were also very well received by the Eclipse Foundation. The Eclipse Foundation develops the Eclipse Platform, which is the open-source



# Software [Continued]

infrastructure on which NiCE is based. The Eclipse Foundation was kind enough to re-publish four of the videos for on their YouTube channel, doubling our view count and exposing us to more of the Eclipse Community than we would normally meet on our own.

The authors would like to acknowledge the support and assistance of the SHARP team at Argonne National Laboratory, most especially Justin Thomas, without which this work would not have been possible.

See the videos **HERE**.

**URL: http://niceproject.sourceforge.net/**

# Awards

### CSMD ANNUAL AWARDS - 2013

### Most Distinguished Scientific Paper

*Thomas Maier: "d-wave pairing from spin fluctuations in the KxFe2-ySe2 superconductors", Thomas A. Maier, S. Graser, P.J. Hirshfeld, D.J. Scalapino, Phys. Rev. B. 83, 100515 (2011).*

This work was led by Thomas Maier and used a fluctuation exchange approximation and a five-orbital tight-binding description of the band structure (made possible because of the ability of the ORNL-based DCA+ software and HPC at OLCF), to calculate the effective pairing interaction for recently discovered superconductors in the KFe2Se2 family.

### Most Distinguished Software

*Team of Jeff Vetter, Anthony Danalis, Gabriel Marin, Collin McCurdy, Jeremy Meredith, Philip Roth, Kyle Spafford, Vinod Tipparaju, Lukasz Wesolowski, and Aditya Sarwade: "The Scalable HeterOgeneous Computing (SHOC) Benchmark Suite".*

The Scalable HeterOgeneous Computing (SHOC) benchmark suite is a collection of benchmark programs testing the performance and stability of systems using heterogeneous computing devices with non-traditional architectures for general purpose computing.

SHOC has been used on systems scaling up to 1000s of devices, like Keeneland and Titan, down to individual hosts, like laptops. Our team is currently developing new versions of SHOC for Intel Xeon Phi and OpenACC. A variety of companies and other researchers have used, recommended, and contributed to SHOC; these include Intel, AMD, ARM, and NVIDIA. The SHOC paper has received 119 citations, and the SHOC software, since its inception, has been downloaded more than 10,000 times, for use in procurements, benchmarking, computer science investigations, education, and other activities.

### Most Significant Technical Contribution

*Eric Lingerfelt for his work related to the development of isotopes.gov and the National Isotope Development Center (NIDC) Online Management Toolkit (OMT).*

The effort has brought significant new funding to National Isotope Development Center (NIDC) at Oak Ridge National Laboratory.

A new, custom-built, database-driven website, isotopes.gov, has been designed and developed for the National Isotope Development Center (NIDC). The NIDC is the sole federal government source of stable- and radio-isotope products for science, medicine, security and applications. Since going live in May 2011, isotopes.gov has provided customers detailed information concerning NIDC activities, funding opportunities, jobs and training, meetings and workshops, outreach and education, production research, and the Isotope Business Office (IBO), which is located here at ORNL. The website also hosts the new Online Catalog of Isotope Products, which allows customers to interactively explore the catalog and submit requests for quotations and new products. Developed by Eric Lingerfelt (CSMD) and Michael Smith (Physics), the website has successfully brought the NIDC's web presence for the forefront and encouraged interaction with new and existing customers. It has also served to educate the public on the important role that isotopes play in society.

# Awards [Continued]

### Special Category

*Rick Archibald was awarded the Special Category award for his work in the utilization of support vector machines (SVMs) to semiautomatically perform endmember extraction from hyperspectral data.*

The strengths of SVM are exploited to provide a fast and accurate calculated representation of high-dimensional data sets that may consist of multiple distributions. Once this representation is computed, the number of distributions can be determined without prior knowledge. For each distribution, an optimal transform can be determined that preserves informational content while reducing the data dimensionality and, hence, the computational cost. Finally, endmember extraction for the whole data set is accomplished. Results indicate that this SVM-based endmember extraction algorithm has the capability of semiautonomously determining endmembers from multiple clusters with computational speed and accuracy while maintaining a robust tolerance to noise.

### INDIVIDUAL AWARDS

### Intern Roisin Langan wins best abstract award at student poster session

Roisin Langan, an intern at Oak Ridge National Laboratory (ORNL), spent last summer improving the ability of climate models to predict the variability and extremes of precipitation. With guidance from her mentors, Richard Archibald and Kate Evans of ORNL's Climate Change Science Institute, Langan analyzed data generated on the Oak Ridge Leadership Computing Facility's Titan supercomputer. Her project, titled "Stochastic Representation of Unresolved Processes in Climate Models," garnered attention lab wide, winning the best abstract award at ORNL's Research Alliance in Math and Science (RAMS) banquet, a student poster session held August 8. Research in this field could result in more accurate warning systems for extreme events, such as flooding, droughts, and heat waves, and help stakeholders plan economic and humanitarian relief efforts. "This experience helped me gain invaluable networking channels, experience, and instruction in effective scientific communication," said Langan, a recent graduate of the University of California, Santa Barbara. Now an intern through ORNL's Nuclear Engineering Science Laboratory Synthesis program, she hopes to enter a graduate program in computational science in fall 2014. - Jennifer Brouner

### Jay Billings – CCSD Outstanding Mentor Award

Jay Jay Billings was honored as the CSMD Outstanding Mentor of the Year (2013). Jay was selected from among several CSMD staff members nominated by interns they mentored during 2013, and was honored along with Outstanding Mentors from each the other divisions in the Computing and Computational Sciences Directorate.

# New Staff

### Stuart Slattery

Stuart is a research staff member in the Computational Engineering and Energy Sciences Group. While completing his Ph.D. in Nuclear Engineering at the University of Wisconsin, Stuart spent two summers at ORNL working with the Consortium for Advanced Simulation of Light-Water Reactors (CASL). During one of those summer internships, Stuart developed the DataTransferKit (DTK), a library for massively parallel multiphysics data transfer based on the concept of geometric rendezvous. Openly available via GitHub (https://github.com/CNERG/DataTransferKit), DTK has become a core component of CASL's Virtual Environment for Reactor Analysis (VERA). Stuart's dissertation topic was "Massively Parallel Monte Carlo Methods for Discrete Linear and Nonlinear Systems", and he is working on one of the ASCR Resilient Extreme-Scale Solvers (RX-Solvers) projects, as well as continuing to contribute to CASL, in part by supporting and extending DTK. In his free time, Stuart enjoys running and rock climbing.

### Megan Cason

Megan Cason is currently working on projects with the Future Technologies Group. In particular, she is working on new tools to characterize and study the behavior of large scale scientific applications. This work intersects with efforts at multiple DOE labs to understand application behavior through proxy applications in order to codesign applications and systems for the next generation of scientific supercomputing. Megan's work also includes investigations into next generation middleware and runtime systems which will enable applications to make better use of the rapidly increasing level of hardware parallelism in high performance computing systems.



# New Staff [Continued]

### Dan Lu

Dan Lu received her Ph.D. in computational science from Florida State University in 2012. Dan comes to the Lab from a position with the U.S. Geological Survey. Dan's background is environmental engineering and hydrological modeling. She is interested in inverse modeling and uncertainty quantification such as assessment of parameter, model and scenario uncertainty. Currently Dan is working on uncertainty quantification part of a LDRD project.

# Community Service

- Hasan Abbasi, Posters Committee Member, SuperComputing 2013 - Denver
- David Bernholdt, reviewer, Oak Ridge Leadership Computing Facility's Director's Discretion program
- David Bernholdt began serving as Technical Project Officer for Intel's project in the Design Forward program
- David Bernholdt, panelist, "Careers in HPC" session of the "Experiencing HPC for Undergraduates" program at SC13
- David Bernholdt, reviewer, Computing in Science and Engineering
- David Bernholdt, reviewer, DOE Advanced Scientific Computing Research Small Business Innovation Research program
- David Bernholdt, reviewer, 28th International Parallel and Distributed Processing Symposium
- David Bernholdt, reviewer, Software: Practice and Experience
- Christian Engelmann, general co-chair, 13th International Conference on Algorithms and Architectures for Parallel Processing (ICA3PP), Vietrisul Mare, Italy, December 16-24, 2013
- Christian Engelmann, technical program committee chair, 4th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (ScalA), at 26th IEEE/ACM International Conference on High Performance Computing, Networking, Storage and Analysis (SC), Denver, CO, USA, November 18, 2013
- Christian Engelmann, technical program committee member, 22nd Euromicro International Conference on Parallel, Distributed and network-based Processing (PDP), Turin, Italy, February 12-14, 2014
- Christian Engelmann, Posters Committee Member, SuperComputing 2013 - Denver
- Manjunath Gorentla Venkata, Programm Commitee Member, 28th IEEE International Parallel and Distributed Processing Symposium.
- Oscar Hernandez, Workshops Committee Member, SuperComputing 2013 - Denver
- Chung-Hsing Hsu, panelist, the 4th Annual EE HPC WG Workshop at SC'13.
- Chung-Hsing Hsu, co-chair, BoF on Total Power Usage Effectiveness at SC'13.
- Chung-Hsing Hsu, session chair, the SC'13 technical paper program.
- Tomislav Janjusic, reviewer, 28th IEEE International Parallel & Distributed Processing Symposium
- Scott Klasky, Technical Papers - Storage, Visualization & Analytics Committee Member, SuperComputing 2013 - Denver
- Gary Liu, member, technical program committee member, IEEE International Conference on Communications (ICC) 2014
- Arthur Maccabe, Technical Papers - System Software Committee Member, SuperComputing 2013 - Denver
- Tiffany Mintz, ACM SRC Student Poster Selection Committee Member, SuperComputing 2013 – Denver
- Thomas Naughton, reviewer, IEEE Transactions on Dependable and Secure Computing.
- George Ostrouchov, Committee chair, SC workshop on Big Data Analytics (BDAC) 2013
- Sarah Powers, FY14 Householder selection committee member, ORNL.
- Sarah Powers, technical reviewer for a RNSD Level-3 milesone report.
- Sarah Powers, session chair (CS and OR Interface session), INFORMS annual conference, Minneapolis, MN, 6-9 October 2013.
- Nageswara Rao, associate editor, International Journal of Distributed Sensor Networks, renewed appointment
- Nageswara Rao, program committee member, The Fourth Workshop on Design, Modeling and Evaluation of Cyber Physical Systems, 2014
- Nageswara Rao, program committee member, 17th International Conference on Information Fusion, 2014
- Nageswara Rao, program committee member, Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (ScalA), 2013
- Philip C. Roth, BoFs Chair, SuperComputing 2013 - Denver
- Phil Roth, Posters Committee Member, SuperComputing 2013 - Denver
- Philip C. Roth, Technical Papers - Performance, Analysis & Tools (PAT) Committee Member, SuperComputing 2013 - Denver
- Pavel Shamis, reviewer, 28th IEEE International Parallel & Distributed Processing Symposium
- Geoffroy Vallee, reviewer, 4th International Conference on Cloud Computing and Services Science

# Community Service [Continued]

- Jeffrey Vetter, ACM Gordon Bell Prize Committee Member, SuperComputing 2013 – Denver
- Jeffrey Vetter Emerging Technologies Committee Member, SuperComputing 2013 - Denver
- Jeffrey Vetter, Panels Committee Member, SuperComputing 2013 – Denver
- Patrick Worley, Technical Papers - Algorithms Committee Member, SuperComputing 2013 – Denver

### Indo-US Workshop

Bobby Philip, CEES/CSMD who is serving as a High Performance Computing Liaison for ORNL in India helped organize an "Indo-US Workshop on High Performance Computing, Applications, and Big Data Analytics[2], that was held during Dec.15-18, 2013 at the Indian Institute of Science (IISc), Bangalore, India. The Indo-US workshop was organized by ORNL (lead: Jeff Nichols) and IISc (leads: Prof N. Balakrishnan and Prof. R. Govindarajan) and was supported by the Indo-US Science and Technology Forum (IUSSTF) as well as corporate sponsors including Intel, Cray, Nvidia, and Lockheed Martin. The aim of the workshop was to promote collaborative research programs in High Performance Computing between Indian educational and research institutes, and U.S. educational and research institutions. The focus areas of the workshop were:

1. HPC systems design involving heterogeneous accelerators, energy efficient HPC systems, software tools and techniques for exascale HPC systems,
2. Computational materials modeling including multiphysics and multiscale modeling/length-scale bridging,
3. Climate modeling for ultra-high resolution using state-of-the-art multi-scale earth system models (ESM) that can support impacts assessment & decision-making,
4. Biological and biomedical systems, and
5. Energy technologies, and data-intensive computing including novel model-free data analysis and visualization, expert systems.

There were roughly 20 U.S. participants and 50 Indian participants from national laboratories, academia, and industry from across both nations.

In addition the ORNL delegation met with the heads of Centers for Development of Advanced Computing (C-DAC) and visited the Fourth Paradigm Institute (CSIR4PI) of the Council for Scientific and Industrial Research (CSIR) in India to discuss potential opportunities for collaboration.

### Fall 2013 Meeting of the Electrochemical Society (ECS)

ORNL CAEBAT team had a strong presence at the ECS Fall meeting. The ORNL team presented the following three papers:

1. "Optimization of Tab Placement in Li-Ion Battery Using Multi-Physics Simulations," S Allu, W Elwasif, S Pannala, S Kalnaus, S Simunovic, and JA Turner, ECS Meeting Abstracts, Oct. 2013
2. "Understanding the Effect of Temperature Gradients in Modules On Cell Balance Using Coupled Multi-Physics Modeling approach," S Pannala, S Allu, W Elwasif, S Kalnaus, S Simunovic, JA Turner, ECS Meeting Abstracts, 1229-1229, Oct. 2013
3. "Three dimensional thermal, electrical and electrochemical modeling of Li-ion batteries," S Kalnaus, S Allu, W Elwasif, S Simunovic, S Pannala, JA Turner, ECS Meeting Abstracts, 1210-1210, Oct. 2013

The first paper presented by S. Allu studied the role of tab placement on reducing the peak temperature of cell by utilizing the optimization/parameter capability within OAS. The second paper presented by S. Pannala looked the imbalance in the cells of a module under different boundary conditions as well as aging conditions. The third paper looked at the application of the OAS framework for coupled electrochemical-thermal-electrical simulations and the effect of swapping out different electrochemical components.

### CSMD Battery Simulation Group Hosts EERE Program Manager

On Nov. 5-6, 2013, DOE EERE [1] Vehicle Technologies Program Manager David Howell visited ORNL. As part of his visit, the ORNL CAEBAT [2] team (Sreekanth Pannala, Srdjan Simunovic, Wael Elwasif, Sergiy Kalnaus, Jay Jay Billings, Taylor Patterson, and CEES Group Leader John Turner) were able to meet with him to demonstrate progress in simulation capabilities, including an initial demonstration of the use of the NEAMS Integrated Computational Environment (NiCE) with OAS [3].

[1] DOE Office of Energy Efficiency and Renewable Energy (EERE)
[2] The Computer-Aided Engineering for Batteries (CAEBAT) program (http://www.nrel.gov/vehiclesandfuels/energystorage/caebat.html) is funded through the Vehicle Technologies (VT) program office within the EERE. This program, led by NREL and including industry and university partners, is developing computational tools for the design and analysis of batteries. CSDM staff are leading development of the shared computational infrastructure used across the program.
[3] http://sourceforge.net/apps/mediawiki/niceproject/index.php?title=CAEBAT

### Software Productivity for Extreme-Scale Science Workshop

The ASCR Workshop on Software Productivity for Extreme-Scale Science (SWP4XS) was held 13-14 January 2014 in Rockville, MD. The meeting was organized by researchers from ANL, LBNL, LANL, LLNL, ORNL (David Bernholdt, CSR/CSMD), and the Universities of Alabama and Southern California at the behest of the US Department of Energy Office of Advanced Scientific Computing Research, to bring together computational scientists from academia, industry, and national laboratories to identify the major challenges of large-scale application software productivity on extreme-scale computing platforms.

The focus of the workshop was on assessing the needs of computational science software in the age of extreme-scale multicore and hybrid architectures, examining the scientific software lifecycle and infrastructure requirements for large-scale code development efforts, and exploring potential contributions and lessons learned that software engineering can bring to HPC software at scale. Participants were asked to identify short- and long-term challenge of scientific software that must be addressed in order to significantly improve the productivity of emerging HPC computing systems through effective scientific software development processes and methodologies.

The workshop included more than 70 participants, including ORNL researchers Ross Bartlett (CEES/CSMD), Al Geist (CTO/CSMD), Judy Hill (SciComp/NCCS), Jeff Vetter (FT/CSMD), in addition to organizer Bernholdt. Participants contributed 35 position papers in advance of the workshop, and the workshop itself included 19 presentations, a panel discussion, and three sets of breakout sessions, most of which are archived on the workshop's web site (http://www.orau.gov/swproductivity2014/)

An outcome of the workshop will be a report that articulates and prioritizes productivity challenges and recommends both short- and long-term research directions for software productivity for extreme-scale science.

# New Funding

### Robust Network Fusion Algorithms for Detection and Localization of Radiation Sources

*Principal Investigator: Nageswara Rao*
*Funding Source: Domestic Nuclear Defense Office*

In support of national defense, Domestic Nuclear Detection Office's (DNDO) Intelligent Radiation Sensor Systems (IRSS) program developed networks of radiation counters for detecting, localizing and identifying low-level, hazardous radiation sources. Tests and analyses of these networks revealed unexpected levels of complexity and challenges in (a) extracting focused information from the extensive measurement data, and (b) developing robust network fusion algorithms necessary for practical scenarios, such as urban environments, border crossings, highways and public events. Under previous Department of Energy and Department of Defense projects, ORNL has developed a foundational theory and experimental methods that overcome several of the limitations of current network fusion algorithms by using a radically new localization-driven, selective-subnet fusion approach, which forms the basis of the algorithms in this project. This project addresses the design, analysis and testing of the next generation network fusion algorithms to achieve robust performance for detection and localization.

# Events

### CSMD Seminars

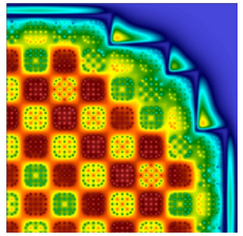
- Adam Larios: New Techniques for Large-Scale Parallel Turbulence Simulations at High Reynolds Numbers
- Tuoc Van Phan: Some Aspects in Nonlinear Partial Differential Equations and Nonlinear Dynamics
- Rich Lehoucq: A Computational Spectral Graph Theory Tutorial
- Jingwei Hu: Fast algorithms for quantum Boltzmann collision operators
- Jeongnim Kim: Analysis of QMC Applications on Petascale Computers
- Terry Haut: Advances on an asymptotic parallel-in-time method for highly oscillatory PDEs
- Galen Shipman: The Compute and Data Environment for Science (CADES)
- Wei Ding: Klonos: A Similarity Analysis-Based Tool for Software Porting in High-Performance Computing
- Chao Yang: Numerical Algorithms for Solving Nonlinear Eigenvalue Problems in Electronic Structure Calculation
- Christian Straube: Simulation of HPDC Infrastructure Attributes

# Events [Continued]

- Surya R. Kalidindi: Data Science and Cyberinfrastructure Enabled Development of Advanced Materials
- Hermann Härtig: A fast and fault tolerant microkernel-based system for exa-scale computing (FFMK)
- Marta D'Elia: Fractional differential operators on bounded domains as special cases of nonlocal diffusion operators
- Tommy Janjusic: Framework for Evaluating Dynamic Memory Allocators including a new Equivalence Class based Cache-Conscious Dynamic Memory Allocator
- Sophie Blondel: NAT++: An analysis software for the NEMO experiment

### CASL Demonstration of Neutronics Coupled to Thermal-Hydraulics

On 12/30/2013, CASL[1] delivered a significant milestone - a quarter-core simulation of the hot full-power conditions for the TVA Watts Bar Unit 1 nuclear reactor using the nonlinearly-coupled neutronics and thermal-hydraulics (heat transfer and fluid flow) within the Virtual Environment for Reactor Applications (VERA). This capability provides dramatically increased detail over typical approaches, delivering detailed information for individual fuel rods, and is an important step in progress toward the goal of modeling a full reactor core with depletion (changes in isotopics due to fission).



***2D slice of a 3D coupled simulation of the thermal neutron flux distribution in TVA's Watts Bar nuclear reactor core near the midplane. The ORNL SP_N neutronics capability Insilico was coupled to the COBRA-TF subchannel thermal-hydraulics code for a significant CASL milestone.***

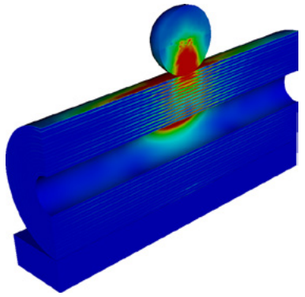
CSMD staff have been key contributors to CASL since its inception, with Computational Engineering and Energy Science (CEES) Group Leader John Turner serving as Chief Computational Scientist and staff from the CEES, Computer Science, and Applied Math groups contributing to CASL goals. For this milestone, Ross Bartlett and Stuart Slattery of CEES played significant roles.

Simulations were performed on approximately 15,000 cores of Titan[2] using a combination of ALCC and INCITE allocations, and would not have been possible without the help of OLCF staff.

[1] http://www.casl.gov/. The Consortium for Advanced Simulation of Light Water Reactors (CASL) was established as the first U.S. Department of Energy (DOE) Innovation Hub, and was created to accelerate the application of advanced modeling and simulation (M&S) to the analysis of nuclear reactors. CASL started operations on July 1, 2010, at its ORNL headquarters in collaboration with ten core partners (Idaho National Laboratory, Los Alamos National Laboratory, Sandia National Laboratories, Electric Power Research Institute, Westinghouse Electric Company, Tennessee Valley Authority, North Carolina State University, University of Michigan, and Massachusetts Institute of Technology). [2] https://www.olcf.ornl.gov/computing-resources/titan-cray-xk7/

### Battery Safety 2013 Conference

On Nov. 15, 2013, CEES Group Leader John Turner presented "Safer Batteries Through Predictive Simulation" at the Battery Safety 2013 conference in San Diego, CA [4]. Although modeling and simulation are typically not emphasized by this community, this well-attended conference provides a forum for publicizing our progress and demonstrating current and potential value.



***Simulation of a cylindrical battery being crushed by a steel ball using ORNL's Virtual Integrated Battery Environment (VIBE), developed as part of the DOE/EERE/VT CAEBAT program. Crushing induces internal short-circuits, which can lead to thermal runaway if not designed properly.***

[1] DOE Office of Energy Efficiency and Renewable Energy (EERE) [2] The Computer-Aided Engineering for Batteries (CAEBAT) program (http://www.nrel.gov/vehiclesandfuels/energystorage/caebat.html) is funded through the Vehicle Technologies (VT) program office within the EERE. This program, led by NREL and including industry and university partners, is developing computational tools for the design and analysis of batteries. CSDM staff are leading development of the shared computational infrastructure used across the program.
[3] http://sourceforge.net/apps/mediawiki/niceproject/index.php?title=CAEBAT
[4] http://www.knowledgefoundation.com/viewevents.php?event_id=301&act=evt

### SimCenter Visit

On Tuesday and Wednesday, December 3-4, 2013, ORNL hosted a visit by research staff from the University of Tennessee at Chattanooga SimCenter, The National Center for Computational Engineering [1] to discuss research interests and expertise and explore potential areas for collaboration. Coordinated by CSMD Computational Engineering and Energy Sciences [2] Group Leader John Turner, the visit included both presentations by SimCenter, ORNL/CSMD, and JICS/NICS [3] staff as well as informal discussions and identification of both active areas for near-term collaboration and areas for potential joint proposal development.

Near-term areas include collaboration on mesh generation challenges of CASL [4], timestepping approaches in climate simulation, advanced modeling and simulation for batteries, and inverse problems and agent-based response, possibly tied to atmospheric dispersion.
Longer-term, it was clear that there are multiple areas of similar interests and complementary expertise that should provide opportunities for collaboration. Institutional and organizational options to facilitate these opportunities were also discussed.

Attendees included:
UTC SimCenter: Tim Swafford, Steve Karman, Jim Newman, Lafe Taylor

ORNL: Jeff Nichols, Barney Maccabe, John Turner, Sreekanth Pannala, Clayton Webster, Rick Archibald, Charlotte Barbier, Mark Berrill, Cory Hauck, Doug Kothe, Mike Leuze, Srdjan Simunovic, Stuart Slattery, Alan Stag, Jack Wells

UTK/JICS/NICS: Glenn Brook, Justin Whitt, Sean Ahern, Dan Stewart

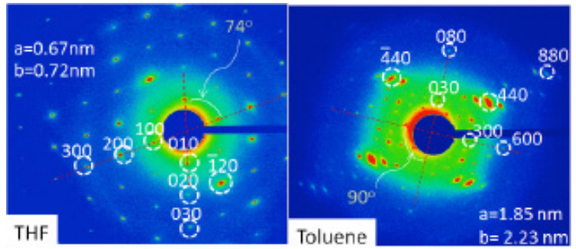
[1] http://www.utc.edu/college-engineering-computer-science/research-centers/simcenter/
[2] http://www.csm.ornl.gov/newsite/cees.html
[3] http://www.jics.utk.edu/
[4] Consortium for Advanced Simulation of Light-Water Reactors (http://www.casl.gov/), a DOE Innovation Hub

# Scientific Achievements

### Solvent-type-dependent polymorphism and charge transport in a long fused-ring organic semiconductor

Chen J, Shao M, Xiao K, Rondinone AJ, Loo YL, Kent PR, Sumpter BG, Li D, Keum JK, Diemer PJ, Anthony JE, Jurchescu OD, Huang J.

Polymorphism is widely encountered in organic solids due to the relatively weak intermolecular interactions (van der Waals type). In this work, we demonstrate that the specific intermolecular interactions between the solvent and aggregated clusters in the initial stage of crystallization can cause a remarkable polymorphism during the solution crystallization of TES ADT. This control over polymorphism is important because crystalline packings/polymorphs of TES ADT when processed at room temperature critically affect device performance, changing the maximum hole mobility by up to 10 times under the same testing conditions.




***Selected area electron diffraction patterns of TES ADT thin films slowly crystallized from THF and toluene solutions in [001] zone.***

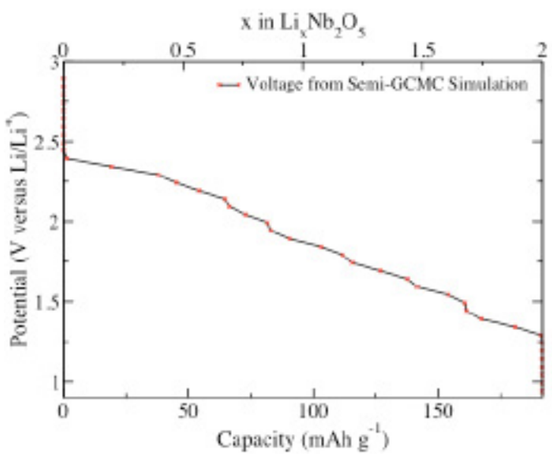
Achievement(s)
- Researchers report a solvent-type-dependent polymorphism of a long fused-ring organic semiconductor and its crucial effects on charge transport. **MORE**
- Researchers show how solvent polarity and intermolecular interactions between the solvent and aggregated clusters in the initial stage of crystallization of a long fused-ring organic semiconductor cause a remarkable polymorphism during the solution crystallization. **MORE**

# Scientific Achievements [Continued]

### Understanding the origin of high-rate intercalation pseudocapacitance in Nb2O5 crystals

Andrew A. Lubimtsev, Paul R. C. Kent, Bobby G. Sumpter and P. Ganesh

Electrochemical energy storage is an essential means of storing/retrieving energy with ubiquitous use in applications from powering portable electronics to vehicular transportation. Our current energy ecosystem demands that we overcome fundamental bottlenecks in materials and design that limit simultaneous high energy density and power-density with long cycle life. The present work highlights a detailed mechanism explaining the origins of high-capacity pseudocapacitance in niobium pentoxide, where local oxidation/reduction reactions occur along with electrostatic charge storage coupled to efficient mass mobility. This new mechanism provides a means for future design/discovery of new energy storage materials with greatly improved energy capacity and very long cycle life.




*Computed CV profile shows a pseudocapacitative slope over the entire range of Li-ion intercalation in Nb2O5.*

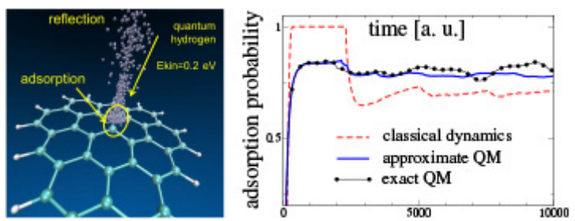
Achievements

- Using first principles calculations, researchers have unravelled a detailed mechanism explaining the high-rate pseudocapacitance in niobium pentoxide. **MORE**
- Using a combination of complementary methods based on the theory of quantum mechanics, researchers have unravelled the principles behind a new mechanism to rapidly increase the amount of energy stored even at very high capacities. **MORE**

### A Quantum Trajectory-Electronic Structure Approach for Exploring Nuclear Effects in the Dynamics of Nanomaterials

Sophya Garashchuk, Jacek Jakowski, Lei Wang, and Bobby G. Sumpter

Quantum behavior of nuclei can play an important role for chemical reactivity and optoelectric properties. We have developed a massively parallel, direct quantum molecular dynamics method and used it to study adsorption of hydrogen/deuterium on a graphene "flake". The colliding atoms are treated as quantum particles whose wavefunction is represented by an ensemble of quantum trajectories (shown as a swarm of particles), moving according to the quantum potential. The electronic potential energy is computed using Self-Consistent Density Functional Theory Tight Binding. Localization of the colliding atomic wavefunction significantly influences the dynamics of the graphene carbons that subsequently alters the adsorption probabilities.




*Above Left: A snapshot of a graphene flake under bombardment by an ensemble of 1000 H atoms. Above Right:Time-dependent adsorption probability of hydrogen on the graphene flake. The results are obtained from classical dynamics, the developed method, and from exact quantum evolution.*

Achievements

- Researchers describe a massively parallel, direct quantum molecular dynamics method that combines a quantum trajectory representation of the nuclear wavefunction discretized into an ensemble of trajectories with an electronic structure description of the electrons. **MORE**
- Using a combination of complementary methods based on the theory of quantum mechanics, researchers have developed a new computational capability to study the dynamics of materials under diverse environmental situations. **MORE**

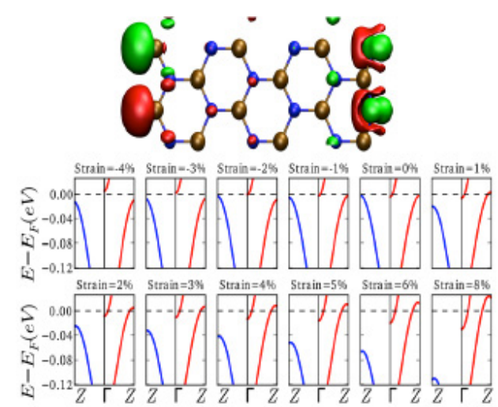


# Scientific Achievements [Continued]

### Spin-resolved self-doping tunes the intrinsic half-metallicity of AlN nanoribbons

Alejandro Lopez-Bezanilla, P. Ganesh, Paul R. C. Kent, Bobby G. Sumpter

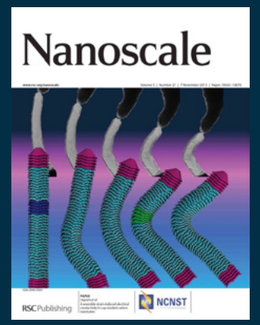
We present a first-principles theoretical study of electric field-and straincontrolled intrinsic half-metallic properties of zigzagged aluminium nitride (AlN) nanoribbons. We show that the half-metallic property of AlN ribbons can undergo a transition into fully-metallic or semiconducting behavior with application of an electric field or uniaxial strain. An external transverse electric field induces a full charge screening that renders the material semiconducting. In contrast, as uniaxial strain varies from compressive to tensile, a spin-resolved selective self-doping increases the half-metallic character of the ribbons. The relevant strain-induced changes in electronic properties arise from band structure modifications at the Fermi level as a consequence of a spin-polarized charge transfer between p-orbitals of the N and Al edge atoms in a spin-resolved self-doping process. This band structure tunability indicates the possibility of designing magnetic nanoribbons with tunable electronic structure by deriving edge states from elements with sufficiently different localization properties. Finite temperature molecular dynamics reveal a thermally stable half-metallic nanoribbon up to room temperature.

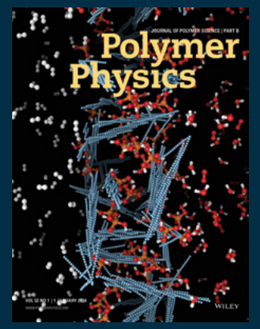



*Top, the real space distribution of the net-spin density corresponding to the electronic states of an AlN nanoribbon ([AlN]6(2)). The red and green isosurfaces correspond to net spin-↑ and spin-↓ electron densities respectively. Bottom, the spin-resolved band structure, within a narrow energy window around the Fermi level for different types/amount of strain.*

Achievements

- Researchers demonstrated how and why the half-metallic property of aluminum nitride (AlN) nanoribbons can undergo a transition to fully-metallic or semiconducting behavior with application of an electric field or uniaxial strain. **MORE**
- Researchers demonstrated that aluminum nitride (AlN) nanoribbons have a rich variety of "on demand" tunable electronic properties due to a spin-resolved self-doping. **MORE**




## Cover Art

An image from the paper "A reversible strain-induced electrical conductivity in cup-stacked carbon nanotubes" by Takuya Hayashi, Thomas C. O'Connor, Katsuhisa Higashiyama, Kohei Nishi, Tomohiro Tojo, Hiroyuki Muramatsu, Yoong Ahm Kim, Bobby G. Sumpter, Vincent Meunier, Mauricio Terrones, and Morinobu Endo was used for the cover of the journal Nanoscale (DOI: 10.1039/C3NR01887C) (top).

For the cover of the journal Polymer Physics (DOI: 10.1002/polb.23403) (above), an image from the paper "A Comparative Study of Phosphoric Acid-doped m-PBI Membranes" by Kelly A. Perry, Karren L. More, E. Andrew Payzant, Roberta A. Meisner, Bobby G. Sumpter, Brian C. Benicewicz has been used.

# Publications and Presentations

### Abstract - conference

- "Block Preconditioners for Fully Implicit Atmospheric Climate Simulation in CAM-SE" Lott, P Aaron (Lawrence Livermore National Laboratory (LLNL)); Woodward, Carol (Lawrence Livermore National Laboratory (LLNL)); Evans, Katherine J. (ORNL), 2013
- "Building on Lessons Learned From Over a Decade of MRNet Research and Development" Miller, Barton P. (University of Wisconsin, Madison); Arnold, Dorian C (University of New Mexico, Albuquerque); Brim, Michael J. (ORNL); Roth, Philip C. (ORNL); Samanas, Evan (University of Wisconsin, Madison); Welton, Benjamin (University of Wisconsin, Madison); Williams, Bill (University of Wisconsin, Madison), 2013
- "Control-Plane Software Methods for High-Performance Network Experiments: UltraScience Net Case Study" Rao, Nageswara S. (ORNL), Cyber Security Expo, 2013
- "Infrastructure resilience using cyber-physical game-theoretic approach: Simplified discrete smart grid infrastructure models, Workshop on Smart Grid," Rao, N.S.V., abstract published, October 17, 2013
- "Developing a power measurement framework for cyber-defense" Hernandez, Jarilyne (Oak Ridge Institute for Science and Education (ORISE)); Pouchard, Line Catherine (ORNL); McDonald, Jeffrey Todd (ORNL), Eight Cyber-security and Information Intelligence Workshop, 2013
- "Stochastic Parameterization for Extreme Precipitation" Langan, Roisin T. (ORNL); Archibald, Richard K. (ORNL); Mahajan, Salil (ORNL); Ricciuto, Daniel M. (ORNL); Yang, Cheng-En (ORNL); Mei, Rui (ORNL); Mao, J. (Oak Ridge National Laboratory (ORNL)); Shi, Xun (ORNL), AGU, 2013
- "Three dimensional thermal, electrical and electrochemical modeling of Li-ion batteries" Kalnaus, Sergiy (ORNL); Allu, Srikanth (ORNL); Elwasif, Wael R. (ORNL); Simunovic, Srdjan (ORNL); Pannala, Sreekanth (ORNL); Turner, John A. (ORNL), 224th ECS Meeting, 2013

### Book (author)

- "Architectural Techniques For Managing Non-volatile Caches " Mittal, Sparsh (ORNL), Lambert Academic Publishing (LAP), 978-3-659-46253-5, Saarbrücken Germany, 2013
- "Cache Energy Optimization Techniques For Modern Processors " Mittal, Sparsh (ORNL), Scholars' Press,978-3-639-51736-1, Saarbrücken Germany, 2013

### Book chapter or article

- "On the Use of the Polynomial Annihilation Edge Detection for Locating Cracks in Beam-Like Structures" Saxena, Rishu (ORNL); Surace, Cecilia (Politecnico di Torino); Archibald, Richard K. (ORNL), 114, 113-83, Elsevier ,London United Kingdom, 2013

### Journal article

- "A Generalized Stocastic Collocation Approach to Constrained Optimization for Random Data Identification Problems" Webster, Clayton G. (ORNL); Gunzburger, Max D. (ORNL), Numerical Methods for Partial Differential Equations, N/A, N/A, 1, 0749-159X, 2013
- "A Parallel EM Algorithm for Model-Based Clustering Applied to the Exploration of Large Spatio-Temporal Data" Chen, Wei-Chen (ORNL); Ostrouchov, George (ORNL); Pugmire, Dave (ORNL); Prabhat, (Lawrence Berkeley National Laboratory (LBNL)); Wehner, Michael (Lawrence Berkeley National Laboratory (LBNL)), Technometrics, 55, 4, 513-523, 1537-2723, 2013
- "A reversible strain-induced electrical conductivity in cup-stacked carbon nanotube" Hayashi, T (Shinshu University); Morokuma, Keiji (ORNL); Meunier, Vincent (ORNL); Meunier, V. (Rensselaer Polytechnic Institute (RPI)); Terrones Maldonado, Mauricio (ORNL); Muramatsu, H (Shinshu University); Sumpter, Bobby G. (ORNL); Kim, Y A (Shinshu University), Nanoscale, 5, 21, 10212, 2040-3364, 2013
- "A Survey of Architectural Techniques For Improving Cache Power Efficiency" Mittal, Sparsh (ORNL), Sustainable Computing: Informatics and Systems, N/A, N/A, 1, 2210-5379, 2013
- "An adaptive sparse-grid-based iterative ensemble Kalman filter approach for parameter field estimation" Gunzburger, Max D. (ORNL); Webster, Clayton G. (ORNL); Zhang, Guannan (ORNL), International Journal of Computer Mathematics, N/A, N/A, 1, 1029-0265, 2013
- "An Adaptive Wavelet Stochastic Collocation Method for Irregular Solutions of PDEs with Random Input Data" Gunzburger, Max D. (ORNL); Webster, Clayton G. (ORNL); Zhang, Guannan (ORNL), Lecture Notes in Computer Science and Engineering, N/A, N/A, 1, 1439-7358, 2013
- "Contribution of the Electron-Phonon Coupling to the Pairing Interaction in LiFeAs" Jishi, R A (California State University); Scalapino, Douglas (University of California, Santa Barbara), Physical Review B, 88, N/A, 184505, 1098-0121, 2013
- "First principles local stress in crystalline and amorphous metals" Egami, Takeshi (University of Tennessee (UTK) and Oak Ridge National Laboratory (ORNL)); Ojha, Madhusudan (Oak Ridge National Laboratory (ORNL)); Nicholson, Don M. (ORNL), Journal of Physics: Condensed Matter, 25, 43, 435505, 0953-8984, 2013
- "Increasing power conversion efficiency of coherent beam combining high power broad-area laser diode array with an optimized V-shaped external Talbot cavity " Liu, Bo (ORNL); Braiman, Yehuda (ORNL), Optics Express, 21, 25, 31218, 1094-4087, 2013
- "Modeling and Characterization of the Magnetocaloric Effect in Ni2MnGa Materials" Nicholson, Don M. (ORNL); Odbadrakh, Khorgolkhuu (ORNL); Shassere, Benjamin (ORNL); Rios, Orlando (ORNL); Hodges, Jason P. (ORNL); Ludtka, Gerard Michael (ORNL); Porter, Wallace D. (ORNL); Sefat, A. S. (Oak Ridge National Laboratory (ORNL)); Rusanu, Aurelian (ORNL); Brown, Greg (ORNL); Evans III, Boyd Mccutchen (ORNL), International Journal of Refrigeration, 37, N/A, 289, 0140-7007, 2013
- "Molecular Dynamics Simulations of Graphene Oxide Frameworks" Zhu, Pan (Rensselaer Polytechnic Institute (RPI)); Sumpter, Bobby G. (ORNL); Meunier, V. (Rensselaer Polytechnic Institute (RPI)); Nicolai, Adrien (Rensselaer Polytechnic Institute (RPI)), Journal of Chemical Theory and Computation, 9, 11, 4890-4900, 1549-9618, 2013
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- "An Efficient Surrogate Modeling Approach in Bayesian Uncertainty Analysis" Zhang, Guannan (ORNL); Gunzburger, Max D. (ORNL); Lu, Dan (ORNL); Webster, Clayton G. (ORNL); Ye, Ming (Florida State University, Tallahassee), ICNAAM 2013 AIP Conference Proceedings, N/A, N/A, 1, 11TH INTERNATIONAL CONFERENCE OF NUMERICAL ANALYSIS AND APPLIED MATHEMATICS - 2013
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- "Computation and volume rendering of large-scale EOF coherent modes in rotating turbulent flow data" Ostrouchov, George (ORNL); Pugmire, Dave (ORNL); Rosenberg, Duane L. (ORNL); Chen, Wei-Chen (ORNL); Pouquet, Annick G. (ORNL), AGU Fall Meeting, 2013
- "Coupled Multi-Physics Model for Li-ion Battery Cells during Impact" Allu, Srikanth (ORNL); Pannala, Sreekanth (ORNL); Kalnaus, Sergiy (ORNL); Elwasif, Wael R. (ORNL); Turner, John A. (ORNL), EUROMAT 2013 , European Congress and Exhibition on Advanced Materials and Processes, 2013
- "DOIs and Supercomputing" Jones, Terry R. (ORNL); Vazhkudai, Sudharshan S. (ORNL); Fuller, Douglas (ORNL), DataCite 2013, 2013
- "Extensions to the Shaping Directive", C. Kartsaklis, D. Bernholdt, M. Eisenbach, O. Hernandez and J. Wayne, presented

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- "Extensions to the Shaping Directive: HPCCG Mini-app", C. Kartsaklis, D. Bernholdt, M. Eisenbach, O. Hernandez and J. Wayne, presented to the OpenACC committee, December 2013
- "Improving HPC Scheduling using Predictive Analytics" Powers, Sarah S. (ORNL); Poole, Stephen W. (ORNL), INFORMS Annual Meeting, 2013
- "Leadership Computing at ORNL: More than a Machine" Bernholdt, David E. (ORNL), HPC Connection Workshop @ SC13, 2013
- "Nanostructured Materials: What's next and How Can Computational Science Help?," B. Sumpter, Materials Science and Physics Seminar, Rensselaer Polytechnic Institute, 2013
- "Optimization of Tab Placement in Li-ion Battery using Multi-Physics Simulations" Allu, Srikanth (ORNL); Elwasif, Wael R. (ORNL); Pannala, Sreekanth (ORNL); Kalnaus, Sergiy (ORNL); Simunovic, Srdjan (ORNL); Turner, John A. (ORNL), ECS, 2013
- "Preliminary Benchmarking results for High-Performance Simulations of Plasma Facing Components with Xolotl" Billings, Jay Jay (ORNL), APS Division of Plasma Physics Annual Meeting, 2013
- "Recent Strategies and Challenges for Simulation and Reproducibility in Climate Modeling" Evans, Katherine J. (ORNL), 2013
- "Safer Batteries Through Predictive Simulation" Turner, John A. (ORNL); Allu, Srikanth (ORNL); Elwasif, Wael R. (ORNL); Kalnaus, Sergiy (ORNL); Pannala, Sreekanth (ORNL); Simunovic, Srdjan (ORNL), Battery Safety 2013, 2013
- "Semantic Challenges and Opportunities in DataONE" Pouchard, Line Catherine (ORNL), International Semantic Web conference, 2013
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- "Xolotl-PSI: Code Development, Testing and Uncertainty Quantification Approaches" Billings, Jay Jay (ORNL); Bernholdt, David E. (ORNL); McCaskey, Alex (ORNL); Belt, Andrew P. (ORNL); Yamaguchi-Phillips, Taro J. (ORNL), SciDAC Annual Review, 2013

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- "Framework for Evaluating Dynamic Memory Allocators including a new Equivalence Class based Cache-Conscious Dynamic Memory Allocator" Janjusic, Tommy (ORNL), 2013
- "How The OLCF Can Benefit From DOIs" Jones, Terry R. (ORNL); Vazhkudai, Sudharshan S. (ORNL); Fuller, Douglas (ORNL), 2013
- "Improving data discovery for DataONE" Pouchard, Line Catherine (ORNL), 2013
- "Modeling and Simulation for Advanced Manufacturing: Challenges and Opportunities" Turner, John A. (ORNL); Babu, Prof. Sudarsanam Suresh (University of Tennessee, Knoxville (UTK)); Blue, Craig A. (ORNL); Dehoff, Ryan R. (ORNL); Pannala, Sreekanth (ORNL); Simunovic, Srdjan (ORNL), 2013
- "Modeling and Simulation Made NiCE!" Billings, Jay Jay (ORNL); Deyton, Jordan H. (ORNL), 2013
- "Quantitative Modeling of Data Structure Vulnerability With an Application-Centric Approach" Li, Dong (ORNL), 2013
- "Strategies for using high- resolution global climate models to characterize weather patterns" Evans, Katherine J. (ORNL), 2013
- "Toward Exascale Resilience with A Data-Centric Approach" Li, Dong (ORNL), 2013
- "Using NiCE with VERA" Billings, Jay Jay (ORNL); Deyton, Jordan H. (ORNL), 2013
- "Xolotl Code Development and Third-Party Library Discussion" Billings, Jay Jay (ORNL), 2013
- "Xolotl: Code Development, Testing and Uncertainty Quantification Approaches" Billings, Jay Jay (ORNL)



# 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
- Computational Engineering and Energy Sciences - John Turner
- Computational Mathematics - Clayton Webster
- 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.

## Contact Information


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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**

OAK RIDGE National Laboratory