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CSMD

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Upcoming Events

21st International Symposium on High Performance Interconnects HotI 2013
(August 21-22)
IEEE Hot Interconnects is the premier international forum for researchers and developers of state-of-the-art hardware and software architectures and implementations for interconnection networks of all scales, ranging from multi-core on-chip interconnects to those within systems, clusters, and data centers.

Fourth International Workshop on Parallel Software Tools and Tool Infrastructures (Oct. 1-4)
The advent of multicore and manycore systems requires that programmers understand how to design, write and debug parallel programs effectively. The increased complexity of multi-threaded parallel programming on multicore platforms requires more insight into program behavior, and necessitates the use of tools that can support programmers in migrating existing software to multicore platforms, and in writing new multi-threaded parallel software. Programmers need increasingly sophisticated methods for instrumentation, measurement, analysis and modeling of applications. To help software developers embrace the multicore revolution, we need both sophisticated tools to support parallel software development, and an extensible tool infrastructure that promotes integration of existing and new tools, and simplifies information exchange and access.

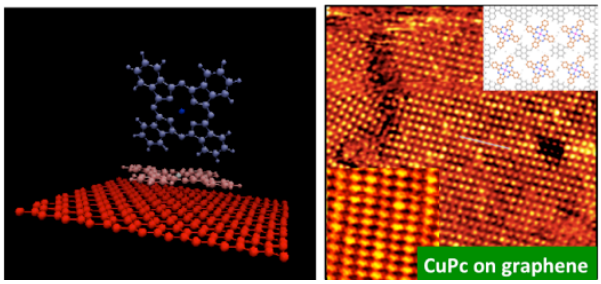
Highlights

Surface-Induced Orientation Control of CuPc Molecules for the Epitaxial Growth of Highly Ordered Organic Crystals on Graphene

ORNL researchers were part of a team that showed how graphene is able to direct the assembly of copper phthalocyanine (CuPc) molecules into epitaxially-aligned superstructures relevant to organic electronics. Theoretical modeling of the mechanisms responsible for this alignment revealed that van der Waals interactions and interfacial dipole interactions induced by charge transfer both play important roles.

This work provides a fundamental understanding of molecular interactions at interfaces important to controlling the nanoscale morphology and orientation of organic semiconductors and to improving optoelectronic processes for high-performance organic electronic devices. Here, graphene is demonstrated to effectively template CuPc molecules to nucleate, orient, and pack in the face-on orientation, the ideal structure for high-performance organic photovoltaics.

Reference:
"Surface-Induced Orientation Control of CuPc Molecules for the Epitaxial Growth of Highly Ordered Organic Crystals on Graphene"



(a) Theoretical modeling of CuPc molecules interactions with graphene in both face-on and side-on orientations (b) STM image of CuPc molecules aligned in the face-on orientation on graphene. Bottom left inset is a higher magnification STM image, top right inset schematically shows the molecular orientation.

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OAK RIDGE National Laboratory

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Modeling and Simulation Made NiCE

(Reprinted with permission from the NEAMS Quarterly Update)

It is often the little things – input or compiler flags, unfamiliar file formats, cryptic output – that make users pause before embracing new scientific software. The big things – modeling and simulation tools that run at unprecedented physical scales and resolution – might never be appreciated by the decision-makers and analysts for whom they were made without taking care of those little things that matter to the user experience. The high-performance computing (HPC) experts cannot be the only people using HPC codes if they are going to have any impact outside the NEAMS community.

The NEAMS program recognized this problem early and commissioned the development of a user-friendly integrated environment. This environment must encapsulate and abstract those activities that do not directly produce a simulation but nonetheless must be performed by users to benefit from the state-of-the-art capabilities provided by the developers. In other words, a simplified yet sophisticated user environment is an important NEAMS objective. After all, users should not have to worry about specialized file formats, runtime flags, long-term data storage, or other in-depth details of how a NEAMS product is installed, configured, and executed. Rather, users should be free to think mainly about what they want to study with NEAMS tools.

Making NiCE

The NEAMS Integrated Computational Environment – NiCE for short – is the NEAMS program's answer to the need for easy usability, accessibility, and collaboration. It complements both SHARP and MOOSE from the reactors and fuels product lines with common tools for creating input files, launching jobs locally and remotely, looking at data in 3D, and managing "assets," such as simulation input and output files.

The primary technical challenges for NiCE are manipulating the large amounts of data that high-fidelity simulations generate and both the physical scale and computational scale (i.e., number of processors) with which it will interact. The NEAMS products are petascale simulators with the potential to generate petabytes of data and run on hundreds of thousands of processing cores. NiCE must, in turn, be an extremely optimized environment that also supports those users who do not have access to the largest of machines or who want to branch out to public or private clouds; arguably, cloud users will comprise the lion's share of the user base.

NiCE is a free and open-source product available at niceproject.sourceforge.net and written in Java with a small amount of C++. It is built on the Open Services Gateway Initiative (OSGi) framework's reference implementation (Equinox) and the rest of the widely acclaimed Eclipse platform. NiCE is both component and plug-in based and can be extended to do new things in a matter of minutes. It has plug-ins for visualization: VisIt for mesh-based output and JMonkeyEngine for 3D constructive solid geometries. The Hierarchical Data Format version 5.0 (HDF5) is used for storing information about reactors, and a relational database (Derby) is used for storing transaction data.

The most recent stable version of NiCE is 2.0, which was released on September 28, 2012.

NiCE's Feature Set and Use Cases

The value that integration and coordination provides to analysts, students, and everyday users cannot be overstated. NiCE enables users from a variety of communities to access NEAMS products uniformly and greatly simplifies training requirements for professionals or students who just want to run some simulations instead of developing code.

NiCE's design is based on requirements (user needs) and features (sets of related requirements) gathered from stakeholders and current and potential users. The requirements elicitation process for NiCE started in February 2009, and all the requirements are reviewed regularly, as often as monthly at the beginning of a development cycle. Interviews, surveys, informal discussions, and literature reviews have all been used to develop the set of functional and non-functional requirements for NiCE. (Non-functional requirements describe the qualities of a system, such as stability and scalability, as opposed to functional requirements, which describe the behavior of a system, that is, the operations it is designed to perform.) The interviews and surveys were very carefully planned and executed to remove as much bias as possible from the questions.

The feature set of NiCE is broad and covers both domain (context) and computer science (capability) concerns. The features were initially developed within the NEAMS community; input from other stakeholders was incorporated later. Currently, the NiCE requirements and features comprise the following capabilities:

- Execute simulations on a wide variety of platforms, including HPC machines, and operating systems.

Highlights (continued)

- Provide tooling to set up models for input files, 3D geometries, meshes, materials, or other data for simulations.
- Provide a suite of analysis tools, including visualization, analytics, and data mining tools and algorithms. Provide utilities for performing uncertainty quantification.
- Provide web-, Android-, and Eclipse-based clients that connect to the same server to facilitate "universal access." Support the composition of new applications and workflows from existing codes and tools.
- Support the development of new computing modules in nuclear energy codes.
- Promote interoperability and loose coupling between codes.
- Provide extensive documentation for users and developers.

Some features are still being implemented.

The feature set and the results from requirements gathering interviews were used to develop seven unique use cases, which are formally defined and cover many types of interactions and scenarios between users and the system. These use cases almost completely track to the list of features. Use case is defined here as a description of the interactions between users and the system, the information that passes between the users and the system, and the before and after states of the system that define how it functions. The use cases are managed as formal specifications stored digitally and updated as needed. The use cases and scope of work they cover are as follows:

Run a simulation. Executing and monitoring simulations is often very difficult for users who are newly acquainted with a particular code and sometimes even for experienced users.

Set up a model. Specifying the input parameters that are necessary to simulate a physical system is a natural partner to executing a simulation and can be a very challenging task. In addition to supporting interactive parameter specification, NiCE includes a graphics editor for visual modification of 3D geometries (Fig. 5).

Analyze data. Many HPC codes provide "raw" results that are not of immediate use to an analyst. NiCE includes a dedicated "reactor analyzer" tool, which is customized for the sort of data created by a reactor simulation and can more quickly provide high-quality 3D visualizations. Mesh variables can be viewed with VisIt, and averages, such as average power per pin, can be visualized on maps at the core, assembly, and pin levels. These capabilities allow users to get to their information faster.

Create an application. Since applications and tools do not always exist to address the exact questions of an analyst, it is often necessary to create new applications, tools, or workflows by combining existing tools or developing completely new tools. NiCE is designed to help users with these tasks.

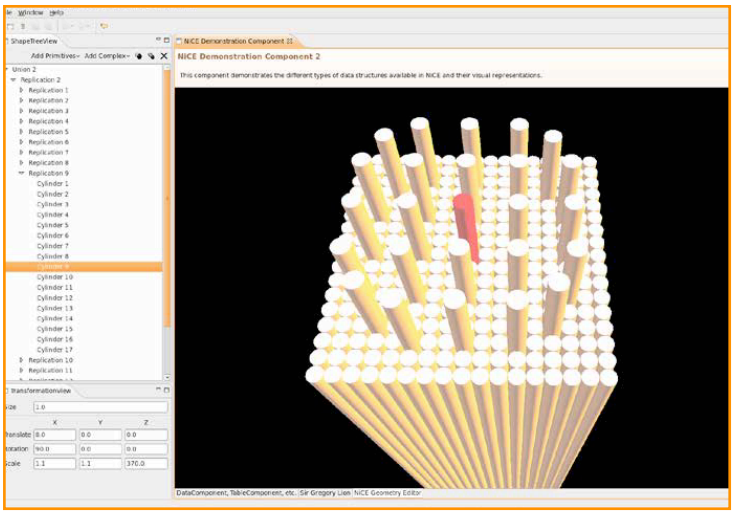


Fig. 5. NiCE geometry editor.

Create a module. NiCE will provide tools for extending existing NEAMS codes so that developers can easily add new modules to the product lines (via tools such as Stork for MOOSE, for example). New modules are based on existing NEAMS simulators and extend their functionality with new physics or different solvers.

Save an asset. NiCE is designed to work with software and data repositories, generically defined as catalogs, to provide both a way to share different assets between users and to store simulations and other files as needed to meet regulatory requirements, promote code re-use, etc.

Search the catalog. Since searching for a particular asset is different task than storing it and often includes retrieval, NiCE has a second data management use case specifically for searching the catalog. Separating searching from submission allows the development team to focus on the unique issues associated with viewing and retrieving data.

The features that enable these uses all point to a system that is more than a set of scripts, more than a user interface or a collection of user interfaces, and more than a file management system. They collectively describe a combined workflow and data management system that couples simple but directed input with advanced 3D visualization, execution of large complex jobs with easily accessed and analyzed output files, and performance of very complicated tasks with the ease of use of a Linux workstation or Windows PC.

Where Will NiCE Be Next?

Last year, development focused on creating the NiCE infrastructure and tools required to provide the features to enable the envisioned uses. The scope of work this year is

directed at deploying NiCE for SHARP- and MOOSE-based applications, starting with BISON. The next stable release of NiCE will include persistence support via a relational database, a web client, and a revamped version of the NiCE tool set for analyzing data from reactor and fuel simulations (i.e., the reactor analyzer). The next release will also include the first versions of the fuels product line plug-ins to NiCE for users that want to set up and launch BISON jobs and limited support for other MOOSEbased applications.

Many capabilities are already available in the "nightly builds" of NiCE that can be found at the Sourceforge project page and are available to anyone who wants to try them out. However, some capabilities will remain limited while they are still in development. Feedback from test use is welcome and wanted because it allows the team to improve the product. Users can report a bug through the Sourceforge project wiki page, submit questions to the user forum or email the author directly.

The NiCE team is also developing more training videos and tutorials that will appear on the project site and YouTube (www.youtube.com/ user/jayjaybillings) in the coming months. The first NiCE training seminar and webinar is being planned for later this year.

NiCE will be presented in March at EclipseCon 2013, and publications about some of its newer features have been submitted to the 2013 meeting of the American Nuclear Society and the 2nd International Workshop on Analytics for Cyber-Physical Systems.

Some computational scientists outside of NEAMS are finding uses for NiCE, including quantum computing and use in other DOE programs, such as Scientific Discovery through Advanced Computing.

Contributing Authors

The following members of the NiCE Development Team contributed to this article: Andrew Belt, Andrew Godfrey, Mike W. Guidry, S. Forest Hull, Eric J. Lingerfelt, Greg Lyon, Alex McCaskey, Ugur Mertyurek, and Neeti Pokhriyal; A. Belt and M. Guidry are from the Univ. Tennessee at Knoxville, and the other contributors are from ORNL.

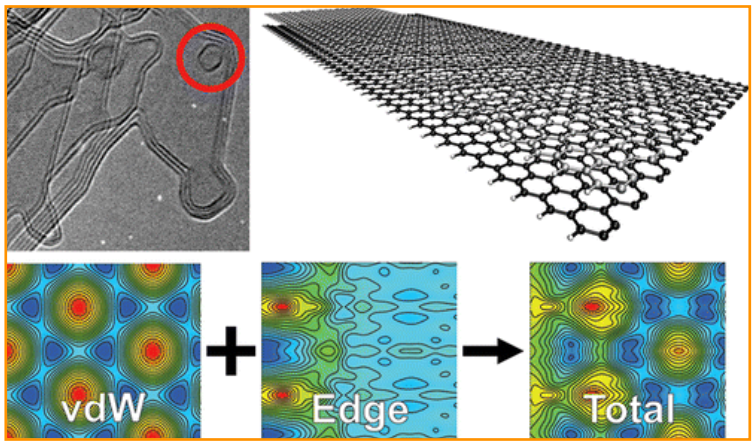
About Jay Jay Billings

Jay Jay Billings is a staff member at in the ORNL Computer Science Research Group and a member of the scientific software team. He holds a master of science degree in theoretical and computational astrophysics from the University of Tennessee. He can be reached by email at billingsjj@ornl.gov or on Twitter at @jayjaybillings

Edge–Edge Interactions in Stacked Graphene Nanoplatelets

CSMD researcher Bobby Sumpter was part of a team whose work on graphene platelets was published in the American Chemical Society's ACSNano Journal.

The team used high-resolution transmission electron microscopy studies to show the dynamics of small graphene platelets on larger graphene layers. The platelets move nearly freely to eventually lock in at well-defined positions close to the edges of the larger underlying graphene sheet. While such movement is driven by a shallow potential energy surface described by an interplane interaction, the lock-in position occurs via edge–edge interactions of the platelet and the graphene surface located underneath. Here, the team quantitatively studied this behavior using van der Waals



Intrinsic stacking interactions of small graphene platelets cause modifications in the local environment of larger graphene plates. Ramifications include: limiting the epitaxial growth of a platelet or arresting the reconstruction of an edge during combined Joule heating and electron irradiation experiments.

density functional calculations. Local interactions at the open edges are found to dictate stacking configurations that are different from Bernal (AB) stacking. These stacking configurations are known to be otherwise absent in edge-free two-dimensional graphene. The results explain the experimentally observed platelet dynamics and provide a detailed account of the new electronic properties of these combined systems.

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The Center for Accelerating Materials Modeling

Team members: Jose Borreguero, Olivier Delaire, Monojoy Goswami, Mark Hagen (PI), Vickie Lynch, Andrei Savici, Galen Shipman, and Bobby Sumpter

Great progress has been made in the last decade towards the predictive materials modeling paradigm that lies at the heart of our ability to solve grand scientific challenges. Theoretical and computational advances enable complex problems to be tackled, including the behavior of correlated systems (electron- electron, electron-phonon), nanoscale materials and assemblies, and functional systems without the simplifying characteristic of periodic long-range order. Similarly, experimental capabilities for the characterization of new materials have expanded in speed and resolving power, with a corresponding growth in the rate and volume of the data acquired. Free-electron lasers and next-generation neutron and synchrotron facilities are pushing the limits of the abilities of research teams to interpret experimental results for scientific impact. Research aimed specifically at meshing new capabilities in theory, data management and modeling, and information-intensive characterization is needed in order to harness effectively the power of individual advances to heighten the impact of materials-by-design.
The goal of this research is to break down remaining barriers to the synthesis and characterization of next- generation materials based on predictive theory, and the corresponding use of these results to enhance the accuracy and accessibility of model predictions.

Specifically, our goal is to improve the predictive capability of materials models and significantly accelerate the rate of scientific discovery from experimental data taken at the Spallation Neutron Source (SNS) by integrating modeling into all aspects of the experimental chain. The leading edge of predictive theory is often remote from research groups with expertise in the synthesis and characterization of novel materials, extending the time required to translate prediction to demonstration. Conversely, this separation also hinders the use of important new experimental results in the development and validation of predictive models. Research aimed toward truly closing the gap between prediction and realization is needed in order to gain the optimum advantages presented by developments in both theory and experiments.

To realize the promise of predictive modeling in advancing experimental research it is necessary to use models to predict directly the results of individual experiments, to compare model and experimental results in near-real time, and to establish clearly the relationships between changes in model assumptions or experimental basis and the resulting impact on predicted quantities. This project will establish the Center for Accelerating Materials Modeling (CAMM). CAMM researchers will develop the understanding of experimental methods, theoretical tools and model sensitivity needed to test and validate predictive materials models against experimental results. Platforms developed in this research for computational, data management, and communications capabilities will be made available to the broader scientific community through interactions with user-driven research at DOE-supported user facilities.

The direct use of predictive modeling to guide experimental studies will be pioneered by linking leadership-class computational capabilities with streaming experimental results from ongoing neutron scattering experiments at the Spallation Neutron Source, providing near-real-time feedback from theory and simulation to optimize the information obtained from individual experiments. The initial focus of this project has been the construction and demonstration of one of the core components of the software toolkit. Specifically, this component is the software to refine potential (or force field) models in molecular dynamics (MD) simulations against data from inelastic/quasi-elastic neutron scattering experiments. Ultimately, we will demonstrate this software for two example cases from “soft” and “hard” condensed matter domains, polyethylene oxide (PEO)–acrylic acid (AA) and KTa1-xNbxO3, respectively.

CAMM began work at the start of the first quarter FY2013. Since this time we have completed the design and initial development for version 1.0 of the analysis workflow involving the interaction of the refinement software package (Dakota[1]) with the codes for the molecular dynamics (MD) simulations and the calculation of the dynamic structure factor for the neutron scattering. Workflow management is based on the Kepler[2] scientific workflow management package (developed in research sponsored by the Office of Advanced Scientific Computing Research) to manage the workflow of submitting and monitoring the computing jobs for the various MD simulations and neutron scattering calculations. Initial tests have been successfully performed using Dakaota and Kepler together. For the science demonstration on polyethylene oxide-acrylic acid initial molecular dynamics simulations have been performed to determine the initial equilibration conditions of the model that will need to be performed as a precursor to the refinement against experimental data.

New Faces in CSMD

Jonathan Schrock

Jonathan Schrock earned his Bachelor's degree from Taylor University in mathematics and computer science. While at Taylor University, Jonathan worked on projects for Lockheed Martin. After graduation, Jonathan then went to work for the Department of Defense. Currently, Jonathan is pursuing a Master's degree in mathematics from UTK.

He is a member of the Computer Science Research Group where he is working on the Durmstrang project.

Moving On

Gabriel Marin
Gabriel Marin left ORNL in February 2013. Gabriel joined ORNL in 2009 to work on performance modeling and analysis, and compilers after completing his PhD at Rice. Gabriel accepted a position at the University of Tennessee and he will continue to live in Knoxville.

Kyle Spafford
Kyle Spafford is returning to Georgia Tech to join the PhD program this fall, and, during the summer, he will work for a GPU company based in Atlanta, near Georgia Tech. Kyle joined the Future Tech Group in 2009, and contributed to several projects during his tenure at ORNL including Keeneland, SHOC, and Aspen.

Community Service

- David E. Bernholdt, reviewer for Parallel Computing (PARCO)
- David E. Bernholdt, reviewer for OLCF Director's Discretion Program
- John Cobb served on the Steering committee for the NSF funded workshop "ADVANCED REGIONAL & STATE NETWORKS (ARNS): ENVISIONING THE FUTURE AS CRITICAL PARTNERS IN DATA-DRIVEN SCIENCE" <https://www.mcnc.org/envision/> Held at Internet2 In Washington DC April 18-19, 2013. The invitation-only workshop was envisioned as assembling a small group of thought-leaders to address issues on building awareness and preparedness of the impact of Big data among both the group of advanced regional network providers and the scientific data communities.
- John Cobb presented one of the abbreviated Keynote talks at the "ADVANCED REGIONAL & STATE NETWORKS (ARNS): ENVISIONING THE FUTURE AS CRITICAL PARTNERS IN DATA-DRIVEN SCIENCE" workshop <https://www.mcnc.org/envision/> Held at Internet2 In Washington DC April 18-19, 2013. John's talk was titled "Data Driven Science Requires Advanced, Distributed Analysis" and is available on the workshop site at <https://www.mcnc.org/sites/default/files/Cobb_ARN2_v02.pdf>
- As a member of The George E. Brown, Jr., Network for Earthquake Engineering Simulation (NEES) governing Board, John Cobb participated in the NEES governing board meeting on March 18, 2013.
- John Cobb has been appointed the the research advisory board of the DMPTool project. <https://dmp.cdlib.org/> The DMPtool is an online resource to assist in the development and preparation of data management plans for research projects. It is a guided process document that contains man of the data management requirements for many federal agencies and academic and research institutions. It also used a federated identity system (InCommon) in order to facilitate multi-institutional and multi-agency projects. The DMPTool project is housed at the California Digital Library but the project is a collaboration of eight different universities, research institutions, and digital data projects. The Research advisory board with provide high-level guidance and feedback to the DMPTool on directions and development in application functionality, DMPTool content, community engagement, and the researcher value proposition.
- Christian Engelmann, reviewer, Parallel Computing (PARCO)
- Christian Engelmann, program committee, 13th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid) 2013
- Christian Engelmann, program committee, 2nd International Workshop on Fault-Tolerance for HPC at Extreme Scale (FTXS) 2013
- Christian Engelmann, program committee, 1st Workshop on Solving Problems with Uncertainties 2013
- Kate Evans, mini-symposium organizer, SIAM Southeastern Section, “Computational Strategies for the next generation of global Earth system models,” Knoxville, TN, Mar. 22-24, 2013.
- Kate Evans, mini-symposium co-organizer, SIAM Computer Science and Engineering, “Implicit Solvers for Earth system Applications,” Boston, MA, Feb. 25-Mar. 1, 2013.
- Travis Humble, appointed co-director of the CCSD-sponsored Quantum Computing Institute
- Travis Humble, appointed a joint faculty position with the University of Tennessee Bredesen Center.
- Travis Humble, invited to contribute an article to the IEEE Communication Society Magazine on Quantum Communication.
- Seyong Lee, paper review for International Conference on Supercomputing (ICS)
- Dong Li, program committee member for IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing (CCGrid), 2013
- Dong Li, Workshop chair for International Workshop on High-Performance, Power-Aware Computing (HP-PAC), 2013
- Dong Li, program committee member for International Supercomputing Conference (ISC), 2013.
- Dong Li, program committee member for Power-Aware Computing Track of EUC 2013, the 11th IEEE/IFIP International Conference on Embedded and Ubiquitous Computing
- Dong Li, journal paper review for IEEE Transactions on Parallel and Distributed System (TPDS)
- Dong Li, journal paper review for Journal of Supercomputing
- Dong Li, journal paper review for Cluster Computing
- Philip Roth, program committee, International Conference on Supercomputing (ICS) 2013
- Philip Roth, program committee, 18th International Workshop on High-Level parallel Programming Models and Supportive Environments (HIPS)
- Philip Roth, program committee, Workshop on Large-Scale Parallel Processing (LSPP) 2013
- Geoffroy Vallee, program committee, Fourth International Conference on Cloud Computing, GRIDs, and Virtualization 2013
- Geoffroy Vallee, program committee, 3rd International Conference on Cloud Computing and Services Science (CLOSER) 2013
- Jeffrey Vetter, program committee, ACM Memory System and Performance Conference 2013

Community Service (continued)

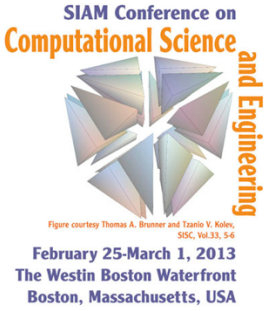
- Jeffrey Vetter, program committee, IEEE International Parallel and DIstributed Systems Symposium, 2013
- Jeffrey Vetter, program committee, ACM GPGPU6 Workshop

SIAM-SES 2013

On March 22-24, Oak Ridge National Laboratory and the University of Tennessee hosted the 37th annual meeting of the SIAM Southeastern Atlantic Section. The meeting included approximately 160 registered participants, of which roughly 60 were students and 20 were from ORNL. There were 4 plenary talks, 24 mini-symposium sessions, seven contributed sessions, and a poster session. Awards were given to students for Best Paper and Best Poster presentations. Attendees were also given guided tours of the Graphite Reactor, the Spallation Neutron Source, and the National Center for Computational Science. The meeting was organized by Chris Baker (ORNL), Cory Hauck (ORNL), Jillian Trask (UT), Lora Wolfe (ORNL), and Yulong Xing (ORNL/UT).

SIAM-CSE13

The CSMD had a strong showing at SIAM-CSE13 with over 25 presentations from staff members from the division. This conference is a leading conference in computer science and mathematics, drawing thousands of researchers from across the globe and supported jointly by NSF and DOE. Division scientist organized eight different mini-symposiums with close to a hundred invited speakers in areas of modern libraries (Christopher Baker), implicit methods for Earth system modeling (Kate Evans), nuclear simulations (Bobby Philip), kinetic theory (Cory Hauck), hybrid architecture linear algebra (Ed D'Azevedo), Resiliency (Jeff Vetter), UQ and stochastic inverse problems (Clayton Webster), and Structural Graph Theory, Sparse Linear Algebra, and Graphical Models (Blair Sullivan).



Durmstrang-2

The semi-annual review for the Durmstrang-2 project was held on March 18-19 in Maryland. Durmstrang-2 is a DoD/ORNL collaboration in extreme scale high performance computing. The long term goal of the project is to support the achievement of sustained exascale processing on applications and architectures of interest to both partners. The Durmstrand-2 project is managed from the Extreme Scale Systems Center (ESSC) of CCSD.

Steve Poole, Chief Scientist of CSMD, presented the overview and general status update at the March review. Benchmarks R&D discussion was facilitated by Josh Lothian, Matthew Baker, Jonathan Schrock, and Sarah Powers of ORNL; Languages and Compilers R&D discussion was facilitated by Matthew Baker, Oscar Hernandez, Pavel Shamis, and Manju Venkata of ORNL; I/O and FileSystems R&D discussion was facilitated by Brad Settlemyer of ORNL; Networking R&D discussion was facilitated by Nagi Rao, Susan Hicks, Paul Newman, and Steve Poole of ORNL ; Power Aware Computing R&D discussion was facilitated by Chung-Hsing Shu of ORNL; System Schedulers R&D discussion was facilitated by Greg Koenig and Sarah Powers of ORNL. The topics of discussion during the executive session of the review included continued funding/growth of the program and development of performance metrics for the project.

APS 2013 March Meeting

The American Physical Society (APS) March Meeting is the largest physics meeting in the world, focusing on research from industry, universities, and major labs. Participation in this years' meeting held in Baltimore, MD (March 18–22, 2013) by staff members of the Computational Chemical and Materials Sciences (CCMS) Group included 24 different talks (bold-face names are from CCMS).

- **Monojoy Goswami, Bobby G. Sumpter**, "Morphology and Dynamics of Ion Containing Polymers using Coarse Grain Molecular Dynamics Simulation," Talk in Session T32: Charged and Ion Containing Polymers (March 21, 2013) APS National Meeting, Baltimore.

- Debapriya Banerjee, Kenneth S. Schweizer, **Bobby G. Sumpter**, Mark D. Dadmun, "Dispersion of small nanoparticles in random copolymer melts," Talk in Session F32: Polymer Nanocomposites II (March 19, 2013) APS National Meeting, Baltimore.

Community Service (continued)

- **Rajeev Kumar, Bobby G. Sumpter**, S. Michael Kilbey II, “00003 Charge regulation and local dielectric function in planar polyelectrolyte brushes,” Talk in Session U32: Charged Polymers and Ionic Liquids (March 21, 2013) APS National Meeting, Baltimore.

- Alamgir Karim, David Bucknall, Dharmaraj Raghavan, **Bobby Sumpter**, Scott Sides, “In-situ Neutron Scattering Determination of 3D Phase-Morphology Correlations in Fullerene -Polymer Organic Photovoltaic Thin Films,” Talk in Session Y33: Organic Electronics and Photonics-Morphology and Structure I (March 22, 2013) APS National Meeting, Baltimore.

- Geoffrey Rojas, P. Ganesh, Simon Kelly, **Bobby G. Sumpter**, John Schlueter, Petro Maksymovych,” Molecule/Surface Interactions and the Control of Electronic Structure In Epitaxial Charge Transfer Salts,” Talk in Session U35: Search for New Superconductors III (March 21, 2013) APS National Meeting, Baltimore.

- Geoffrey A. Rojas, P. Ganesh, Simon Kelly, **Bobby G. Sumpter**, John A. Schlueter, Petro Maksymovich, “Density Functional Theory studies of Epitaxial Charge Transfer Salts,” Talk in Session N35: Search for New Superconductors III (March 20, 2013) APS National Meeting, Baltimore.

- Arthur P. Baddorf,Qing Li, Chengbo Han, J. Bernholc, Humberto Terrones, **Bobby G. Sumpter, Miguel Fuentes-Cabrera**, Jieyu Yi, Zheng Gai, Peter Maksymovych, Minghu Pan,” Electron Injection to Control Self-Assembly and Disassembly of Phenylacetylene on Gold,” Talk in Session C33: Organic Electronics and Photonics - Interfaces and Contacts (March 18, 2013) APS National Meeting, Baltimore.

- Mina Yoon, Kai Xiao, Kendal W. Clark, An-Ping Li, David Geohegan, **Bobby G. Sumpter**, Sean Smith, “Understanding the growth of nanoscale organic semiconductors: the role of substrates,” Talk in Session Z33: Organic Electronics and Photonics - Morphology and Structure II (March 22, 2013) APS National Meeting, Baltimore.

- Chengbo Han, Wenchang Lu, Jerry Bernholc, **Miguel Fuentes-Cabrera**, Humberto Terrones, **Bobby G. Sumpter,** Jieyu Yi, Zheng Gai, Arthur P. Baddorf, Qing Li,. Peter Maksymovych, Minghu Pan, “Computational Study of Phenylacetylene Self-Assembly on Au(111) Surface,” Talk in Session C33: Organic Electronics and Photonics - Interfaces and Contacts (March 18, 2013) APS National Meeting, Baltimore.

- Jaron Krogel, **Jeongnim Kim**, David Ceperley “Prospects for efficient QMC defect calculations: the energy density applied to Ge self-interstitials,” Talk in Session J24: Quantum Many-Body Systems and Methods I (March 19, 2013) APS National Meeting, Baltimore.

- Kendal Clark, **Xiaoguang Zhang**, Ivan Vlassiouk, Guowei He,Gong Gu, Randall Feenstra, An-Ping Li, “Mapping the Electron Transport of Graphene Boundaries Using Scanning Tunneling Potentiometry,” Talk in Session G6: CVD Graphene - Doping and Defects (March 19, 2013) APS National Meeting, Baltimore.

- Gregory Brown, **Donald M. Nicholson**, Markus Eisenbach, **Kh. Odbadrakh** “Wang-Landau or Statistical Mechanics,” Talk in Session G6: Equilibrium Statistical Mechanics, Followed by GSNP Student Speaker Award (March 18, 2013) APS National Meeting, Baltimore.

- **Don Nicholson, Kh. Odbadrakh**,German Samolyuk, G. Malcolm Stocks,” Calculated magnetic structure of mobile defects in Fe,” Session Y16: Magnetic Theory II (March 22, 2013) APS National Meeting, Baltimore.

- **Khorgolkhuu Odbadrakh, Don Nicholson**, Aurelian Rusanu, German Samolyuk, Yang Wang, Roger Stoller, **Xiaoguang Zhang**, George Stocks, “Coarse graining approach to First principles modeling of structural materials,” Session A43: Multiscale modeling--Coarse-graining in Space and Time I (March 18, 2013) APS National Meeting, Baltimore.

- **M. G. Reuter** & P. D. Williams, "The Information Content of Conductance Histogram Peaks: Transport Mechanisms, Level Alignments, and Coupling Strengths" Talk in Session R43: Electron Transfer, Charge Transfer and Transport Session, (March 20,2013) APS National Meeting, Baltimore.

- **Paul R. C. Kent,** Panchapakesan Ganesh, Jeongnim Kim, Mina Yoon, Fernando Reboredo, "Binding and Diffusion of Li in Graphite: Quantum Monte Carlo Benchmarks and validation of Van der Waals DFT" Talk in Session A5: Van der Waals Bonding in Advanced Materials – Materials Behavior, (March 18, 2013) APS National Meeting, Baltimore.

- Peter Staar, **Thomas Maier**, Thomas Schulthess, "DCA+: Incorporating self-consistently a continuous momentum self-energy in the Dynamical Cluster Approximation" Talk in Session N24, APS National Meeting,Baltimore.

Community Service (continued)

- **Thomas Maier,** Peter Hirschfeld, Douglas Scalapino, Yan Wang, Andreas Kreisel, "Pairing strength and gap functions in multiband superconductors: 3D effects" Talk in Session G37: Electronic Structute Methods II,(March 20, 2013) APS National Meeting, Baltimore.

- **Thomas Maier**, Yan Wang, Andreas Kreisel, Peter Hirschfeld, Douglas Scalapino, "Spin fluctuation theory of pairing in AFe2As2" Talk in Session G37: Electronic Structure Methods II,(March 20, 2013), APS National Meeting, Baltimore.

- Peter Hirschfeld, Andreas Kreisel, Yan Wang, Milan Tomic, Harald Jeschke, Anthony Jacko, Roser Valenti, **Thomas Maier**, Douglas Scalapino, "Pressure dependence of critical temperature of bulk FeSe from spin fluctuation theory" Talk in Session G37: Electronic Structure Methods II (March 20, 2013), APS National Meeting, Baltimore.

- Markus Eisenbach, Junqi Yin, **Don M. Nicholson**, Ying Wai Li, “First principles calculation of finite temperature magnetism in Ni,” Talk in Session C17: Magnetic Theory I (March 18, 2013), APS National Meeting, Baltimore.

- Madhusudan Ojha, **Don M. Nicholson**, Takeshi Egami, “Ab-initio atomic level stresses in Cu-Zr crystal, liquid and glass phases,” Talk in Session G42: Focus Session: Physics of Glasses and Viscous Liquids I (March 19, 2013), APS National Meeting, Baltimore.

- Junqi Yin, Markus Eisenbach, **Don Nicholson**, “Spin-lattice coupling in BCC iron,” Talk in Session T39: Metals Alloys and Metallic Structures (March 21, 2013), APS National Meeting, Baltimore.

- German Samolyuk, Yuri Osetsky, Roger Stoller, **Don Nicholson**, George Malcolm Stocks, “The modification of core structure and Peierls barrier of 1/2$<111>$ screw dislocation in bcc Fe in presence of Cr solute atoms,” Talk in Session T39: Metals Alloys and Metallic Structures (March 21, 2013), APS National Meeting, Baltimore.

Successful workshop on Big Data and High Performance Computing hosted by ORNL in Jekyll Island Georgia

SOS is an invitation-only 2 1/2 day meeting held each year by Sandia labs, Oak Ridge National lab, and Swiss Technical institute. This year it was hosted by ORNL in Jekyll Island Georgia on March 25-28, 2013.

The theme this year was "The intersection of High Performance Computing and Big Data". There were 40 speakers and panelists from around the world representing views from industry, academia, and national laboratories. The first day focused on the gaps between big computing and big data and the challenges of turning science data into knowledge. On the second day the talks and panels focused on where HPC and big data intersect and the state of big-data analysis software. The morning of the third day focused on the politics of big data including the issues of data ownership.

Findings of the meeting include the fact that large experimental facilities such as CERNs Large Hadron Collider, and the new telescopes coming online already generate prodigious amounts of scientific data. The volume and speed that data is generated requires that the data be analyzed on the fly and only a tiny fraction be kept. The amount kept still amounts to many petabytes. The attendees stressed how important provenance is to the use of the archived data by other researchers around the world. The majority of today's scientific data is only of value to the original researcher, because the data lacks the meta-data required for others to use it. The talks and panels clearly showed the intersection of high performance computing and big data. They also showed that the converse is not necessarily true, i.e. big data (as defined by Google and Amazon) does not require high performance computing. These vendors and their customers are able to get their work done on large, distributed networks of independent PCs. The meeting was filled with lively discussion, and provocative questions.

For those wanting to know more, the agenda and talks are posted on the SOS17 website: http://www.csm.ornl.gov/workshops/SOS17/

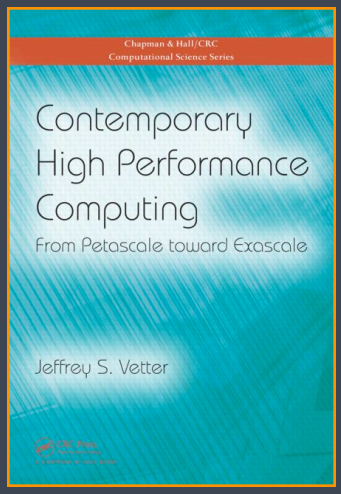
Awards

Federal Laboratory Consortium (FLC) for Technology Transfer 2013 Interagency Partnership Award.
Co-recipient for ORNL contribution to the ForWARN Forest Disturbance Monitoring Project with the U.S. Department of Agriculture Forest Service, NASA Stennis Space Center, and the U.S. Geological Survey EROS Data Center, April 2013.

Events

Seminars and Workshops

SOS 17 Conference
SIAM SEAS 2013 Annual Meeting
J.W. Banks: Stable Partitioned Solvers for Compresible Uid-structure Interaction Problems
Travis Thompson: Navier-Stokes equations to Describe the Motion of Fluid Substances
Bob Salko: Development, Improvement, and Validation of Reactor Thermal-Hydraulic Analysis Tools
Thomas L. Lewis: Finite Difference and Discontinuous Galerkin Numerical Methods for Fully Nonlinear Second Order PDEs with Applications to Stochastic Optimal Control
Charles K. Garrett: Numerical Integration of Matrix Riccati Differential Equations with Solution Singularities
Giacomo Dimarco: Asymptotic Preserving Implicit-Explicit Runge-Kutta Methods For Non-Linear Kinetic Equations
Tom Berlijn: Effects of Disorder on the Electronic Structure of Functional Materials
Joshua D. Carmichael: Seismic Monitoring of the Western Greenland Ice Sheet: Response to Early Lake Drainage
Mili Shah: Calculating a Symmetry Preserving Singular Value Decomposition
Zheng (Cynthia) Gu: Efficient and Robust Message Passing Schemes for Remote Direct Memory Access (RDMA)-Enabled Clusters
Taylor Patterson: Simulation of Complex Nonlinear Elastic Bodies Using Lattice Deformers
Makhan Virdi: Modeling High-resolution Soil Moisture to Estimate Recharge Timing and Experiences with Geospatial Analyses
Roshan J. Vengazhiyil and C. F. Jeff Wu: Experimental Design, Model Calibration, and Uncertainty Quantification
Li-Shi Luo: Kinetic Methods for CFD
Tarek Ali El Moselhy: New Tools for Uncertainty Quantification and Data Assimilation in Complex Systems



Cover Art

Jeffrey Vetter is the editor of *Contemporary High Performance Computing: From Petascale toward Exascale*. The book focuses on the ecosystems surrounding the world's leading centers for high performance computing (HPC). It covers many of the important factors involved in each ecosystem: computer architectures, software, applications, facilities, and sponsors.

Publications/Presentations

Abstract - conference

- Archibald, Richard K. (ORNL), Baker, Christopher G. (ORNL), Evans, Katherine J. (ORNL), Lott, P Aaron (Lawrence Livermore National Laboratory (LLNL)), Ribbeck, Jennifer E. (ORNL), Woodward, Carol (Lawrence Livermore National Laboratory (LLNL)). "Multiscale Methods for Accurate, Efficient, and Scale-Aware Models of the Earth System, Biological and environmental research program review poster session." Biological and environmental research program review poster session, Oak Ridge, Tennessee, 10/2012

- Archibald, Richard K. (ORNL), Branstetter, Marcia L. (ORNL), Evans, Katherine J. (ORNL), Gaddis, Abigail L. (ORNL), Jiang, Tianyu (ORNL), Mahajan, Salil (ORNL), Hebbur Venkata Subba Rao, Vishwas (ORNL). "Analysis of present-day high-resolution Community Atmosphere Model (CAM4) simulations." Biological and environmental research program review poster session, Oak Ridge, Tennessee, 10/2012

- Deiterding, Ralf (ORNL), Poole, Stephen W. (ORNL), Glowinski, R. (University of Houston, Houston). "A Reliable Split-Step Fourier Method for Simulating the Propagation of Ultra-Fast Pulses in Optical Communication Fibers." 8th IMACS Int. Conf. on Nonlinear Evolution Equations and Wave Phenomena: Computation and Theory, Athens, Georgia

- Gorti, Sarma B. (ORNL), Radhakrishnan, Balasubramaniam (ORNL). "Modeling the strength and ductility of magnesium alloys containing nanotwins." 2012 MRS Fall Meeting & Exhibit, Boston, Massachusetts, 11/2012

- Norman, Matthew R. (ORNL), Larkin, Jeff (Cray, Inc.), Archibald, Richard K. (ORNL), Carpenter, Ilene (National Renewable Energy Laboratory (NREL)), Anantharaj, Valentine G. (ORNL). "The Path to Accelerating the Community Atmospheric Model - Spectral Element Dynamical Core on Hybrid Multi-Core Systems." KIAPS2012, Seoul, , 11/2012

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- Radhakrishnan, Balasubramaniam (ORNL), Gorti, Sarma B. (ORNL), Patton, Robert M. (ORNL), Simunovic, Srdjan (ORNL). "Genetic Algorithm Based Multi-Objective Optimization of a Wrought Magnesium Alloy for High Strength and Ductility." MRS Fall Meeting, Boston, Massachusetts, 11/2012

- Radhakrishnan, Balasubramaniam (ORNL), Gorti, Sarma B. (ORNL), Simunovic, Srdjan (ORNL). "Multi-Objective Optimization of Wrought Magnesium Alloy Microstructure for Strength and Ductility." 2nd World Congress on Integrated Computational Materials Engineering, Salt Lake City, Utah

- 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, Maryland, 3/2013

- Zhang, Wen (ORNL), Zhang, Xiaoguang (ORNL), Feng, Zhili (ORNL), Wang, Hsin (ORNL). "Time Domain Elastic Wave Solution of a Driven Thin Plate in Ultrasonic Welding." the SIAM 2013 Annual Meeting, San Diego, California

Publications/Presentations (continued)

Book chapter or article

- Huang, Jingsong (ORNL), Qiao, Rui (Clemson University), Feng, Guang (Clemson University), Sumpter, Bobby G. (ORNL), Meunier, Vincent (ORNL). "Chapter 5. Modern theories of carbon-based electrochemical capacitors." 3/2013

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Edited Book

- Vetter, J.S., Ed., Contemporary High Performance Computing: From Petascale Toward Exascale, 1 ed. Boca Raton: Taylor and Francis, 2013, pp. 750. Publisher, Amazon.

Journal article

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- Kumar, Rajeev (ORNL), Goswami, Monojoy (ORNL), Sumpter, Bobby G. (ORNL), Novikov, Vladimir (ORNL), Sokolov, Alexei P. (ORNL). "Effects of backbone rigidity on the local structure and dynamics in polymer melts and glasses." Physical Chemistry Chemical Physics, 2/2013

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Paper in conference proceedings (book, CD)

- Ding, Wei (University of Houston, Houston), Hernandez, Oscar R. (ORNL), Chapman, Barbara (University of Houston, Houston). " Similarity-Based Analysis Tool for Porting OpenMP Applications." Facing the Multicore-Challenge III, Stuttgart, Germany, 9/2012
- Engelmann, Christian (ORNL). "Investigating Operating System Noise in Extreme-Scale High-Performance Computing Systems using Simulation." 11th IASTED International Conference on Parallel and Distributed Computing and Networks (PDCN) 2013, Innsbruck, Austria
- Hernandez, Oscar R. (ORNL), Poole, Stephen W. (ORNL), Kuehn, Jeffery A. (ORNL), Jana, Siddhartha (University of Houston, Houston), Pophale, Swaroop (University of Houston, Houston), Chapman, Barbara (University of Houston, Houston). "The OpenSHMEM Analyzer." The 6th Conference on Partitioned Global Address Space Programming Models, Santa Barbara, California, USA, 2012
- Ihme, Matthias (University of Michigan), Sun, Yong (University of Michigan), Deiterding, Ralf (ORNL). "Detailed Simulations of Shock-Bifurcation and Ignition of an Argon-diluted Hydrogen/Oxygen Mixture in a Shock Tube." 51st AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition, Grapevine (Dallas/Ft. Worth Region), Texas, USA, 1/2013
- Kartsaklis, Christos (ORNL), Civario, G (Irish Centre for High-End Computing). "A Java Library for the Generation and Scheduling of PTX Assembly." NVIDIA GTC 2009, Santa Clara, California, USA, 2010
- Pokhriyal, Neeti (ORNL), Billings, Jay Jay (ORNL), Mertyurek, Ugur (ORNL), Godfrey, Andrew T. (ORNL). "Anomaly Detection for High Fidelity Core simulators." American Nuclear Society: 2013 Annual Meeting, Atlanta, Georgia, USA
- Pokhriyal, Neeti (ORNL), Mertyurek, Ugur (ORNL), Godfrey, Andrew T. (ORNL), Billings, Jay Jay (ORNL). "Knowledge Discovery from Nuclear Reactor Simulation Data." International Workshop on Analytics for Cyber-physical Systems: Held in conjunction with SIAM Data Mining 2013, Austin, Texas, USA
- Radhakrishnan, Balasubramaniam (ORNL), Gorti, Sarma B. (ORNL), Yan, Yong (ORNL), Clarno, Kevin T. (ORNL). "Phase Field Simulations of Hydride Reorientation in Zircaloys." 2013 International High-Level Radioactive Waste Management Conference, Albuquerque, New Mexico, USA
- Tiwari, Devesh (ORNL), Vazhkudai, Sudharshan S. (ORNL), Kim, Youngjae (ORNL), Ma, Xiaosong (ORNL), Boboila, Simona (Northeastern University), Desnoyers, Peter (Northeastern University). "Reducing Data Movement Cost using Energy-Efficient Active Computation on SSD." HotPower 12: Workshop on Power-Aware Computing and Systems, Hollywood, California, USA 2012
- Weerapurage, Dinesh P. (ORNL), Sullivan, Blair D. (ORNL), Groer, Christopher S. (ORNL). "Parallel Algorithms for Graph Optimization using Tree Decompositions." IPDPS 2013, Boston, Massachusetts, USA 2013

Publications/Presentations (continued)

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- Cardall, Christian Y. (ORNL), Budiardja, R. D. (University of Tennessee, Knoxville (UTK)), Mezzacappa, Anthony (ORNL). "Turbulent magnetic field amplification from spiral SASI modes in core-collapse supernovae." Journal of Physics Conference Series, Gatlinburg, Tennessee, USA 2012

- Elwasif, Wael R. (ORNL), Bernholdt, David E. (ORNL), Pannala, Sreekanth (ORNL), Allu, Srikanth (ORNL), Foley, Samantha S. (ORNL). "Parameter Sweep and Optimization of Loosely Coupled Simulations Using the DAKOTA Toolkit." Proceedings - IEEE 15th International Conference on Computational Science and Engineering, Paphos, , Cyprus 2012

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Presentation material - conference

- 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.

- Baker, Christopher G. (ORNL). "Fast and Reliable Trust-Region Eigensolvers." , SIAM Computational Science and Engineering 2013, Boston, Massachusetts, USA

- Billings, Jay Jay (ORNL), McCaskey, Alex (ORNL), Pokhriyal, Neeti (ORNL), Lingerfelt, Eric J. (ORNL), Guidry, Mike W. (ORNL), Belt, Andrew P. (ORNL), Lyon, Gregory M. (ORNL), Hull, Scott F. (ORNL), Godfrey, Andrew T. (ORNL), Mertyurek, Ugur (ORNL). "Simulate This! - The Eclipse Platform as an Integrated Computational Environment." EclipseCon 2013, Boston, Massachusetts, USA

- Branstetter, Marcia L., Jitendra Kumar, Peter E. Thornton, Benjamin Mayer, Robert Cook, and Michele M. Thornton, “Update on Development of a High Resolution Surface Weather Forcing Dataset for CLM Using NEXRAD and DAYMET,” Land Model Working Group Meeting, Boulder, CO, February 2013.

- Branstetter, Marcia L., Jitendra Kumar, Peter E. Thornton, Benjamin Mayer, Robert Cook, and

- Budiardja, R., Cardall, C., Endeve, E., & Mezzacappa, A., 2013,"GenASiS: An Object-Oriented Approach to High-Performance Multiphysics Code with Fortran 2003,” Poster presented at the 37th Annual Meeting of the SIAM Southeastern Atlantic Section, March 23, 2013

- Endeve, Eirik., "Approaches to Supernova Neutrino Radiation Transport,” talk given at the37th Annual Meeting of the SIAM Southeastern Atlantic Section, Knoxville, Tennessee, March 24, 2013

- McClean, Julie, Dave Bader, Elena Yulaeva, Caroline Papadopoulos, Milena Veneziani, Mathew Maltrud, Phil Jones, Kate Evans, Marcia Branstetter, and Jim Hack, “T85 and T341 Fully-Coupled CESM Simulations: Climatology Comparisons and Present-Day Transient Initialization Strategy,” Ocean Model Working Group Meeting, Boulder, CO, January 2013.

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- Norman, M., J. Larkin, R. Archibald, I Carpenter, and V. Anamtharaj, “The Path to Accelerating the Community Atmospheric Model Spectral Element Dynamical Core on Hybrid Multi-core Systems,” KIAPS International Symposium on Global NWP System Modeling, 2012.

- Reuter, Matthew G. (ORNL). "Exorcising Numerical Ghosts from ab initio Calculations of Electron Transport." SIAM Conference on Computational Science and Engineering, Boston, Massachusetts, USA

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Publications/Presentations (continued)

- Vetter, J.S., “Automated Exploration of the HPC Co-Design Space.” 1st International Workshop on Strategic Development of High Performance Computers, Tsukuba, Japan, 2013
- Vetter, J.S., “Intersection of Big Computing and Big Data.” SOS17, Jekyll Island, Georgia, 2013
- Vetter, J.S., D. Li, and W. Yu, “Classifying Soft Error Vulnerabilities in Extreme-Scale Scientific Applications Using a Binary Instrumentation Tool.” SIAM CSE Conference, Boston, 2013
- Webster, Clayton G. (ORNL), Stoyanov, Miroslav K. (ORNL), FINNEY, Charles E A (ORNL), Pannala, Sreekanth (ORNL), Daw, C Stuart (ORNL), Wagner, Robert M. (ORNL), Edwards, Kevin Dean (ORNL), Green Jr, Johney Boyd (ORNL). "High Dimensional Multiphysics Metamodeling for Combustion Engine Stability." , SIAM CSE 2013, Boston, Massachusetts, USA
- Worley, Patrick H. (ORNL), Evans, Katherine J. (ORNL), Boghozian, Adrianna J. (ORNL). "Analysis of Convergence and Performance Variability for Continental Ice Sheet Modeling at Scale." , SIAM Conference on Computational Science and Engineering, Boston, Massachusetts, USA
- Worley, Patrick H. (ORNL). "Parallel Implementation and Performance of the SEACISM Version of the Community Ice Sheet Model." , SIAM Southeastern Atlantic Section Annual Meeting, Knoxville, Tennessee, USA
- Worley, Patrick., Analysis of Convergence and Performance Variability for Continental Ice Sheet Modeling at Scale (with K. Evans and A. Boghozian), SIAM Conference on Computational Science and Engineering, The Westin Boston Waterfront, Boston, MA, February 26, 2013.
- Worley, Patrick., Capturing Computer Performance Variability in Production Jobs (and other topics), Innovative Computing Laboratory Seminar, University of Tennessee, Knoxville, TN, March 22, 2013
- Worley, Patrick., Katherine Evans, and Adrianna Boghozian. Analysis of Convergence and Performance Variability for Continental Ice Sheet Modeling at Scale, SIAM Conference on Computational Science and Engineering, The Westin Boston Waterfront, Boston, MA, February 26, 2013.
- Xing, Yulong (ORNL). "Energy conserving discontinuous Galerkin methods for the wave propagation problems." , SIAM Conference on Computational Science & Engineering (CSE13), Boston, Massachusetts, USA
- Xing, Yulong (ORNL). "High order accurate RKDG methods for the shallow water equations on unstructured triangular meshes." , SIAM Conference on Computational Science & Engineering (CSE13), Boston, Massachusetts, USA
- Sumpter, Bobby G., “Nanomaterials Theory Institute and Computational Chemical and Materials Sciences,” Duke University, March 12 (2013).
- Zhulin, Igor B., “Evolution of a Complex Signal Transduction System”. Joint Seminars in Molecular Biology. University of California-Davis.

Presentation material - no conference

- Elliott, James J. (ORNL), Webster, Clayton G. (ORNL), Stoyanov, Miroslav K. (ORNL), Mueller, Frank (North Carolina State University). "Quantifying the Impact of Single Bit Flips on Floating Point Arithmetic."
- Worley, Patrick H. (ORNL). "Capturing Computer Performance Variability in Production Jobs (and other topics)."
- Xing, Yulong (ORNL). "Discontinuous Galerkin methods for the wave propagation problems."
- Xing, Yulong (ORNL). "Energy conserving discontinuous Galerkin methods for the wave equations."

Team Profile - Predictive Mathematics

The role of the Predictive Mathematics Team at ORNL is to develop innovative, massively scalable and resilient mathematical and computational approaches for scientific (model) discovery as well as decision-sciences. To address these objectives, we use fundamental mathematics which (i)
for problems that we cannot simulate, improve our simulation capabilities and (ii) for problems we can simulate, apply predictive methodologies with rigorous uncertainty quantification to support decision-makers and for engineering solutions.

Current postdocs include
Diego Galindo (Mentor: Clayton Webster)
Kris Garrett (Mentor: Cory Hauck) and
PhD student Nick Dexter (Advisor: Clayton Webster).

Senior Staff members:
Clayton Webster is an applied mathematician and Team Leader in the PMG at ORNL. He is also jointly appointed as an Professor in the Department of Mathematics at the University of Tennessee and in the Department of Scientific Computing at Florida State University. Clayton received his Ph.D. in Mathematics from FSU in 2007 and is a former John von Neumann Fellow, awarded by the DOE at Sandia National Labs. His research is focussed on uncertainty quantification, stochastic PDEs, high-dimensional approximation theory and numerical and functional analysis. Clayton also serves on the editorial boards of the SIAM Journal on Numerical Analysis, the SIAM Journal on Uncertainty Quantification and the International Journal for Uncertainty Quantification.

Cory Hauck is an applied mathematician with expertise in computational aspects of kinetic theory, hyperbolic partial differential equations, and multi-scale methods. He is a staff member in the PMG at Oak Ridge National Laboratory (ORNL) and Joint Assistance Professor in the Mathematics Department at the University of Tennessee. He received his Ph.D. in applied mathematics from the University of Maryland and, previous to joining ORNL, was a postdoctoral research associate with the Center for Nonlinear Studies and the Computational Physics and Methods Group at Los Alamos. Cory is also a core participant and Oak Ridge node leader for Ki-Net, the NSF-funded research network on "the kinetic description of emerging challenges in multi-scale problems of natural sciences."

Rick Archibald is a staff scientist in the Computational Mathematics group at ORNL. He held the Alston S. Householder Fellowship in Scientific Computing from 2005 until his staff appointment in 2007. Archibald received his PhD in mathematics from the Arizona State University in 2002. Archibald's current research interests include developing uncertainty quantification algorithms for climate models, designing algorithms for the next generation of high-performance architecture, and establishing long-time integration steps for the dynamical core of climate models at high resolution.

Team Profile (continued)

Yulong Xing obtained his Ph.D. in Mathematics from Brown University, and joined ORNL on 2009 as a joint faculty between University of Tennessee and ORNL. His research interests are mainly in numerical analysis and scientific computing. His current research is focused on the design, analysis and implementation of accurate and efficient numerical methods for partial differential equations, more specifically, hyperbolic conservation laws with source terms, and wave propagation problems.

Guannan Zhang is the Householder fellow in the Computer Science and Mathematics Division at ORNL since August 2012. He obtained his Ph.D. degree at the Florida State University in the summer of 2012. Dr. Zhang is currently a member of the Predictive Mathematics Group (PMG) at ORNL. His research is focused on mathematical foundations of uncertainty quantification (UQ), including numerical methods for stochastic partial differential equations, high-dimensional stochastic approximation and discontinuity detection, Data assimilation, stochastic optimization and related applications.

Miro Stoyanov is a Virginia Tech graduate of 2009 form the department of Mathematics. After a two year post-doc assignment at Florida State University, Miroslav joined Oak Ridge National Lab in February of 2012. As of January 2013, Miroslav is an ORNL staff member working int he are of uncertainty quantification. Particular interests include high dimensional interpolation and dimension reduction as well as software resilience with respect to soft hardware errors.

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

OAK RIDGE National Laboratory