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QUARTERLY NEWSLETTER FOR THE COMPUTER SCIENCE AND MATHEMATICS DIVISION

CSMD

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Science Highlights

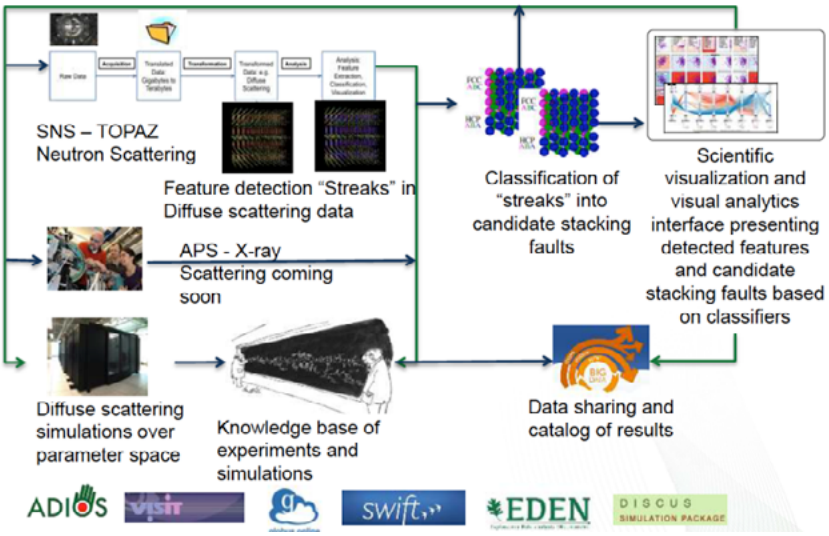
Analysis and Feature Detection in Large Volumes of Diffuse X-ray and Neutron Scattering from Complex Materials

Thomas Proffen, Ray Osborn, Rick Archibald, Stuart Campbell, Ian Foster, Scott Klasky, Tashin Kurc, Dave Pugmire, Michael Reuter, Galen Shipman, Chad Steed, Chris Symons, Ross Whitfield, Doug Fuller, Guru Kora, Mike Wilde, Justin Wozniak

By linking experimental and computational facilities across the DOE, researchers were able to uncover stacking faults in double-layered perovskite, $Sr_3(Ru_{1-x}Mn_x)_2O_7$.

Perovskites are promising materials for solid-state batteries. Understanding the electronic properties of double-layered perovskite requires that defects in perovskite lattice be well understood. The researchers demonstrated how it is possible to use experimental data both from SNS and APS in combination with large libraries of HPC computational simulations of targeted stacking fault geometries to identify details of the volumetric disordering of double-layered perovskite – a critical step to understanding material properties.

Thomas Proffen, Ray Osborn, Rick Archibald, Stuart Campbell, Ian Foster, Scott Klasky, Tashin Kurc, Dave Pugmire, Michael Reuter, Galen Shipman, Chad Steed, Chris Symons, Ross Whitfield, Doug Fuller, Guru Kora, Mike Wilde, Justin Wozniak, "Analysis and Feature Detection in Large Volumes of Diffuse X-ray and Neutron Scattering from Complex Materials", Supercomputing 2015 Abstract [link]. Full presentation at CADES [link]



OAK RIDGE National Laboratory

Science Highlights [Continued]

Glprof: A Gprof inspired, Callgraph-oriented Per-Object Disseminating Memory Access Multi-Cache Profiler

Tomislav Janjusic and Christos Kartsaklis

We introduce a new memory-centric memory trace based tool, Glprof and show through trace examples the importance of Glprof and its ability to breakdown complex data-structure behavior into simple and intuitive summaries.

Understanding how intricate data-structures are accessed and how a given memory system responds is a complex task. Glprof, specifically aims to lessen the burden of the programmer to pinpoint heavily involved data-structures during an application's run-time, and understand data-structure run-time usage. We demonstrated the application of our tool in the context of Spec benchmarks using the Glprof profiler and two concurrently running cache simulators, PPC440 and AMD Interlagos.

Tomislav Janjusic and Christos Kartsaklis, "Glprof: A Gprof inspired, Callgraph-oriented Per-Object Disseminating Memory Access Multi-Cache Profiler", Workshop on Tools for Program Development and Analysis in Computational Science, Held in conjunction with the international Conference on Computational Computing (ICCS 2015)

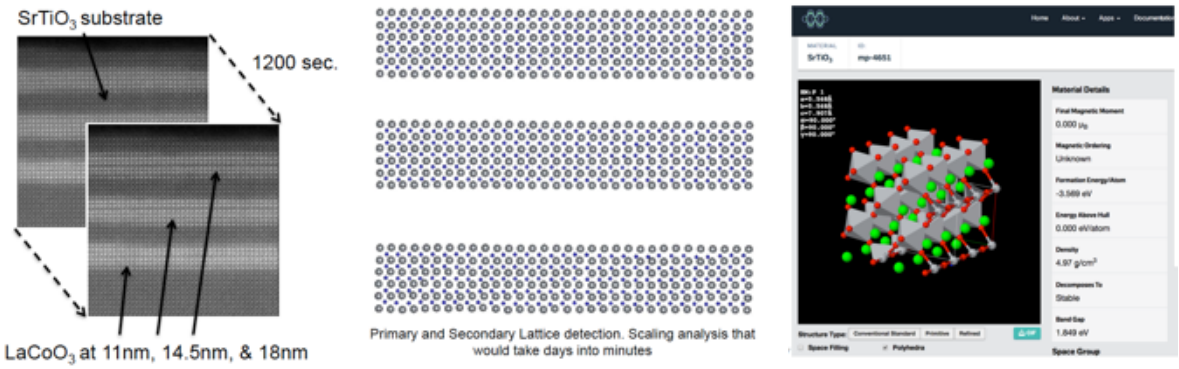
Image Analysis and Feature Classification in Atomically Resolved Images: Genomic Libraries through Smart Data

Sergei Kalinin, Rick Archibald, Alex Belianinov, Albina Borisevich, Miaofang Chi, Eirik Endeve, John Freeland, Doug Fuller, Anubhav Jain, Stephen Jesse, Guruprasad Kora, Nouamane Laanait, Kristin Persson, Amanda Petford-Long, Andrew Lupini, Oleg Ovchinnikov, Galen Shipman, David Skinner, Chris Symons, Ray Unocic

By linking experimental and computational facilities across the DOE, researchers were able to uncover local physical and chemical properties of Perocskite Superlattices.

Perovskites are promising materials for solid-state batteries. Understanding the structural dynamics at an atomic level through direct measurement require statistical analysis of thousands of images that can only reasonably be done on HPC. Feeding this experimentally based analysis of lattice configuration back into the HPC simulation will close the analysis gap, join big computation and big experimentation, allow near-real-time discovery of material properties.

Rick Archibald, Alex Belianinov, Albina Borisevich, Miaofang Chi, Eirik Endeve, John Freeland, Doug Fuller, Anubhav Jain, Stephen Jesse, Sergei Kalinin, Guruprasad Kora, Nouamane Laanait, Kristin Persson, Amanda Petford-Long, Andrew Lupini, Oleg Ovchinnikov, Galen Shipman, David Skinner, Chris Symons, Ray Unocic, "Image Analysis and Feature Classification in Atomically Resolved Images: Genomic Libraries through Smart Data", Supercomputing 2015 Abstract [link]. Full presentation at CSMD [link]



Left: Perocskite Superlattices experimentally measured at CNMS

Center: Dynamics analyzed on TITAN by IFIM team.

Right: Electronic structure of lattice configuration for IFIM analysis calculated by Materials Project on EDISON.

Science Highlights [Continued]

Simulating North American Heat Waves and Large-scale Weather Regimes in Climate Models: Circulation Characteristics and Synoptic-scale Activity

Tianyu Jiang, K. J. Evans, V. Anantharaj, R. Archibald, D. Bader, M. Branstetter, J. Hack, P. Jones, S. Mahajan, M. Maltrud, J. McClean, M Taylor, P. Worley

In this study, the summertime heat waves in North America and the associated ridging/blocking activity are characterized using reanalysis data and global climate models with different horizontal resolutions (~120 km /~30 km) and ocean modules (prescribe/interactive).

The typical synoptic features accompanying the heat waves are depicted. The frequency of occurrence and intensity of the upstream blockings are examined.

The discrepancy between the reanalysis and the models on the heat wave characteristics as well as the upstream blocking activity is assessed by comparing the passage of synoptic-scale transients and its local reinforcement to the anticyclonic circulation. The result indicates: 1) a general agreement on the first moment of climatological distribution with different resolution; 2) the higher resolution model can improve the high-order moments of the atmosphere circulation, including the weather regimes, which is critical to a reliable simulation and projection of the climate extremes.

Dunn-Sigouin, E., and S.-W. Son (2013), Northern Hemisphere blocking frequency and duration in the CMIP5 models, J. Geophys. Res. Atmos., 118, 1179–1188, doi:10.1002/jgrd.50143.

Ngar-Cheung Lau and Mary Jo Nath, 2012: A Model Study of Heat Waves over North America: Meteorological Aspects and Projections for the Twenty-First Century. J. Climate, 25, 4761–4784. doi: http://dx.doi.org/10.1175/JCLI-D-11-00575.1

Tuning Friction at the Nanoscale

Evgheni Strelcov, Rajeev Kumar, Vera Bocharova, Bobby G. Sumpter, Alexander Tselev, and Sergei V. Kalinin

This work demonstrates a way of controlling friction on ionic surfaces at the nanoscale by using electrical stimulation and ambient water vapor. Frictional forces arise whenever objects around us are set in motion. Controlling them in a rational manner means gaining leverage over mechanical energy losses and wear. This paper presents a way of manipulating nanoscale friction by means of in situ lubrication and interfacial electrochemistry. Water lubricant is directionally condensed from the vapor phase at a moving metal-ionic crystal interface by a strong confined electric field, thereby allowing friction to be tuned up or down via an applied bias. The electric potential polarity and ionic solid solubility are shown to strongly influence friction between the atomic force microscope (AFM) tip and salt surface. An increase in friction is associated with the AFM tip digging into the surface, whereas reducing friction does not influence its topography. No current flows during friction variation, which excludes Joule heating and associated electrical energy losses. The demonstrated novel effect can be of significant technological importance for controlling friction in nano- and micro-electromechanical systems.

"Nanoscale Lubrication of Ionic Surfaces Controlled via Strong Electric Field", Evgheni Strelcov, Rajeev Kumar, Vera Bocharova, Bobby G. Sumpter, Alexander Tselev, Sergei V. Kalinin, Scientific Reports 5, 8049 (2015). DOI: 10.1038/srep08049

Schematic diagram showing how electricity and water from air can be used to control friction levels on ionic surfaces. As water forms around the nanoscale electrode (A,B), it allows for further penetration into the sample surface (C), thereby increasing or decreasing friction. Also this approach can enable precise patterning of the surface (E)

Science Highlights [Continued]

Fidelity of Climate Extremes in High Resolution Global Climate Simulations

Mahajan S., K. J. Evans, M. Branstetter, V. Anantharaj and J. K. Leifeld

Precipitation extremes have tangible societal impacts. Here, we assess if current state of the art global climate model simulations at high spatial resolutions (0.35◦x0.35◦) capture the observed behavior of precipitation extremes in the past few decades over the continental US. We design a correlation-based regionalization framework to quantify precipitation extremes, where samples of extreme events for a grid box may also be drawn from neighboring grid boxes with statistically equal means and statistically significant temporal correlations. We model precipitation extremes with the Generalized Extreme Value (GEV) distribution fits to time series of annual maximum precipitation. Non-stationarity of extremes is captured by including a time-dependent parameter in the GEV distribution. Our analysis reveals that the high-resolution model substantially improves the simulation of stationary precipitation extreme statistics particularly over the Northwest Pacific coastal region and the Southeast US. Observational data exhibits significant non-stationary behavior of extremes only over some parts of the Western US, with declining trends in the extremes. While the high-resolution simulations improve upon the low-resolution model in simulating this non-stationary behavior, the trends are statistically significant only over some of those regions.

Mahajan S., K. J. Evans, M. Branstetter, V. Anantharaj and J. K. Leifeld (2015): Fidelity of precipitation extremes in high-resolution global climate simulations, Procedia Computer Science (accepted)

Agent-based Event Simulation at Scale

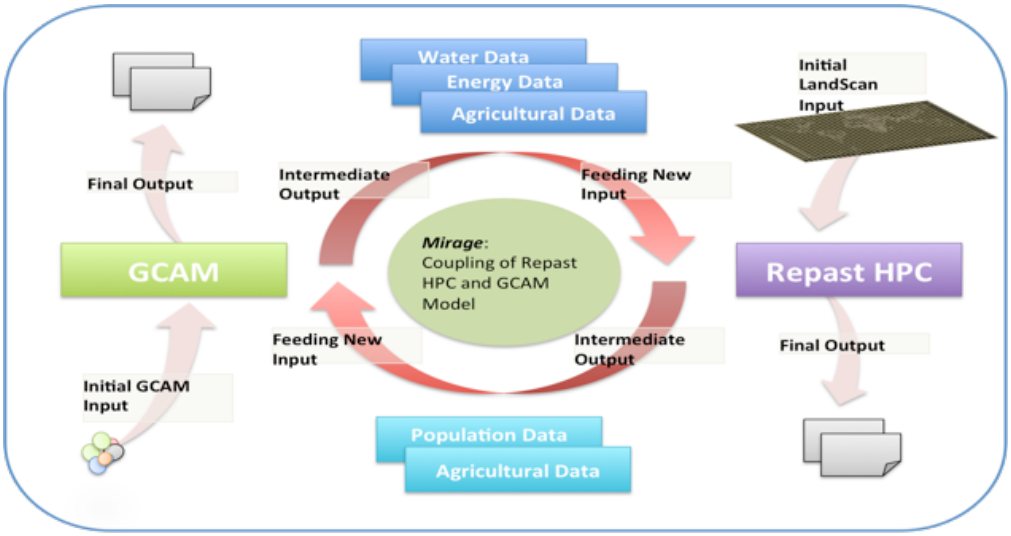
Byung H. Park

Agent-Based Event Simulation Models for Healthcare Ecosystem and Global High-Resolution Collaborative Models implemented on Titan. This implementation demonstrates ORNL's unique capability to simulate ultra scale agent-based discrete event simulation.

The agent-based discrete event simulation model is widely used to simulate the actions and interactions of autonomous agents and assess the aggregated results on the system. As problem sizes increase to include hundred millions or even billions of actors, to simulate dynamics among the actors in response to different social, climate, economical, or environmental inputs requires a whole new paradigm of modeling a large-scale simulation. This work creates one such framework that brings the HPC capability to problems that require high-resolution simulations. Two strategic use cases of the framework have been introduced: healthcare cost simulation and various geospatial related simulation.

Gautam S. Thakur, Byung H. Park, Özgür Özmen, Jack Schryver, Mallikarjun Shankar, and Gilbert G. Weigand, Synthetic Data Generation for High-Fidelity HPC Healthcare Simulation: Beneficiary-Provider Network Example, 2015 Spring Simulation Multi-Conference (SpringSim'15)

Byung H. Park, Melissa R.Allen, Devin White, Eric Weber, John T. Murphy, Michael J. North, and Pam Sydelko, MIRAGE: A framework for data-driven collaborative high-resolution simulation, GeoComputation 2015 Conference.



Data Driven High-Resolution Collaborative Framework: The HPC agent model is coupled with a disparate model(s) to simulate how human population and its environments influence each other.

Science Highlights [Continued]

A Directives API for Loop Transformations

Christos Kartsaklis, EunJung Park, and John Cavazos

We defined the directives API "HSLOT" for transforming and parallelizing loops and implemented it in a production compiler. This allows for the rapid transformation of Fortran loop structures in custom ways and with a programming simplicity similar to OpenMP FOR-loop parallelization.

HSLOT strives to simplify the task of transforming source code in order to test different optimization paths on current and future computing systems. HSLOT arms users with a rich set of configurable transformation directives – these can be used as-they-are, specialized and most importantly combined into powerful, customized, transformations. We offer a plethora of loop transformations, which includes both the classic set (unroll, fuse, fission, tile, and so on) as well as unique ones (specialize, swap nest, split, fork, and so on) that are not found in other state-of-the-art systems. We showed how HSLOT can be used for breaking dependencies and enabling additional optimizations and parallelism, while leaving the original sources intact. Users use HSLOT by simply annotating loops with the transformations sequence and by compiling with our Open64-based HSLOT-implementing

Showcasing one (fuse) of the many supported HSLOT transformation primitives.

Fortran compiler, which produces both object files and optionally source.

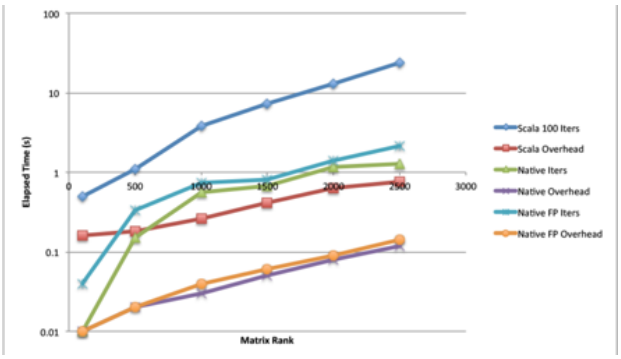
Christos Kartsaklis, EunJung Park and John Cavazos, "HSLOT: the HERCULES scriptable loop transformations engine", 4th International Workshop on Domain-Specific Languages and High-Level Frameworks for High Performance Computing, held in conjunction with the SC14: The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC14)

Functional Programming Computational Cores Embedded Into Traditional High Performance Computing Language Programs

Phil Roth

We demonstrated feasibility of embedding functional programming (FP) computational cores written in Scala into programs written in three traditional languages used to implement high performance computing (HPC) applications: Fortran, C, and C++. Measured the performance and overhead of pilot hybrid FP programs.

To demonstrate the feasibility of constructing hybrid FP applications, we have developed five computational cores in Scala and embedded them into programs written in the three traditional languages for implementing HPC applications: Fortran, C, and C++. Because Scala programs are executed on a JVM, we embedded a JVM in Fortran, C, and C++ demonstration frame programs using the C-language JNI. We added calls to each Scala FP core within each demonstration frame program. Because the JNI is a C language API, invoking the Scala FP cores from C and C++ was relatively easy. Because Fortran and Scala use substantially different in-memory data representations and calling conventions, we developed an automated tool for generating wrapper functions that handle conversions between the two languages' data representations. We used a five-point stencil FP core to measure the performance and overhead of a hybrid FP program to an iterative implementation of the same stencil operation and an FP implementation



Performance and overhead of Scala/Fortran hybrid stencil application compared to traditional Fortran iterative and FP implementations.

using a traditional HPC language. We found the hybrid FP implementation had a substantial performance gap with the iterative and traditional FP implementations, and our measurements suggested that the overhead of constructing a JVM and converting data representations for the Scala FP core were primary contributors to this gap. In this sense, our hybrid FP programs are similar to GPU-accelerated programs, in that much work must be done in GPU kernels to amortize the cost of initializing the GPU device and transferring data to and from the GPU to the frame program.

Funding for this work was provided by the Office of Advanced Scientific Computing Research, U.S. Department of Energy. The work was performed at Oak Ridge National Laboratory (ORNL).

Science Highlights [Continued]

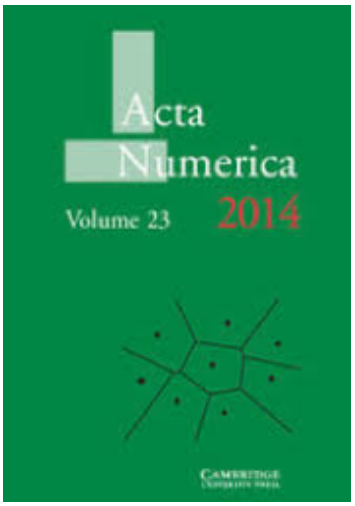
REVIEWS: Stochastic FEMs for PDEs with random data

Max Gunzburger, Clayton Webster, and Guannan Zhang

A generalized stochastic finite element framework is established in which methods such as Monte Carlo, stochastic Galerkin and collocation are described and compared from both a theoretical and computation perspective.

The quantification of probabilistic uncertainties in the outputs of physical, biological, and social systems governed by partial differential equations with random inputs require, in practice, the discretization of those equations. Stochastic finite element methods refer to an extensive class of algorithms for the approximate solution of partial differential equations having random input data, for which spatial discretization is effected by a finite element method. Fully discrete approximations require further discretization with respect to solution dependences on the random variables. For this purpose several approaches have been developed, including intrusive approaches such as stochastic Galerkin methods, for which the physical and probabilistic degrees of freedom are coupled, and non-intrusive approaches such as stochastic sampling and interpolatory-type stochastic collocation methods, for which the physical and probabilistic degrees of freedom are uncoupled. All these method classes are surveyed in this article, including some novel recent developments.

Funding for this work was provided by the Office of Advanced Scientific Computing Research, U.S. Department of Energy. The work was performed at Oak Ridge National Laboratory (ORNL).



Publication Covers

Related Publications:

M. Gunzburger and C. Webster, Uncertainty Quantification for partial differential equations with stochastic coefficients. To appear: The Mathematical Intelligencer, 2015.

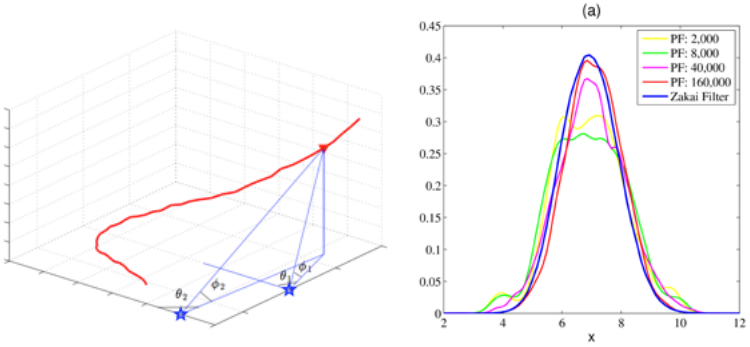
M. Gunzburger, C. Webster and G. Zhang, Stochastic finite element methods for partial differential equations with random input data. Acta Numerica, 521-650, 2015.

EQUINOX: A hybrid sparse-grid approach for nonlinear filtering

F. Bao, Y. Cao, C. Webster, and G. Zhang

A hybrid finite difference algorithm for the Zakai equation is constructed to solve nonlinear filtering problems. The algorithm combines the splitting-up finite difference scheme and hierarchical sparse grid method to solve moderately high dimensional nonlinear filtering problems. When applying hier- archical sparse grid method to approximate bell-shaped solutions in most applications of nonlinear filtering problem, we introduce a logarithmic approximation to reduce the approximation errors. Some space adaptive methods are also introduced to make the algorithm more efficient. Numerical experiments are carried out to demonstrate the performance and efficiency of our algorithm.

Funding for this work was provided by the Office of Advanced Scientific Computing Research, U.S. Department of Energy. The work was performed at Oak Ridge National Laboratory (ORNL).



(Left) The problem of interest: bearing-only tracking; (Right) Comparison of marginal distributions of the dynamical state process obtained by particle filters (PFs) and our approach. It shows that PFs need 160,000 samples to achieve similar accuracy as our approach with about 2,300 sparse grid points.

Related Publications:

F. Bao, Y. Cao, C. Webster, and G. Zhang, A hybrid sparse-grid approach for nonlinear filtering problems on adaptive-domain of the Zakai equation approximation. SIAM J. on Uncertainty Quantification, 2, 784 – 804, 2014.

Software

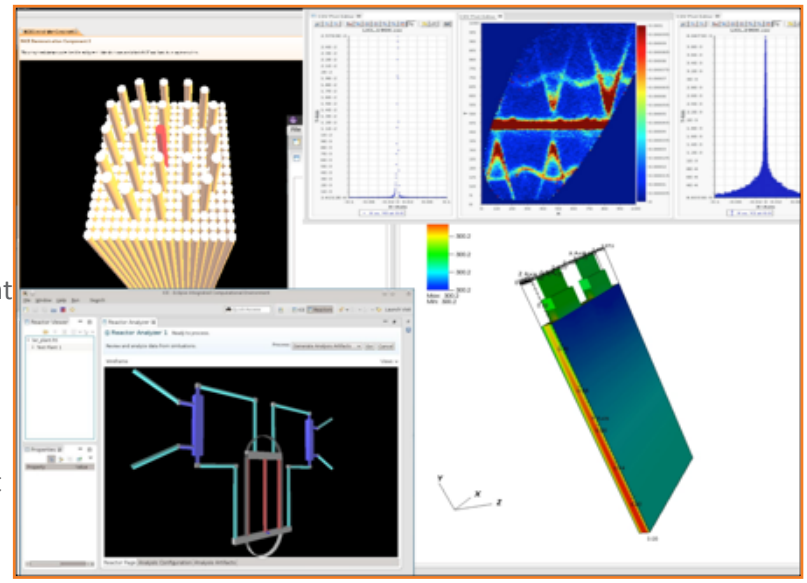
Upgrading Modeling and Simulation with the Eclipse Integrated Computational Environment

Jay Jay Billings, Alexander J. McCaskey, Andrew Bennett, Jordan H. Deyton, Hari Krishnan, Taylor Patterson, Anna Wojtowicz

Researchers have taken the tools in Eclipse that are used for authoring scientific software and repurposed them for using scientific software.

The result is the Eclipse Integrated Computational Environment (ICE); a general purpose, easily extended M&S platform that significantly updates the way computational scientists interact with their software. It improves productivity and streamlines the workflow for computational scientists when they need to create input files, launch jobs on local or remote machines, and process output. Since it is based on the Eclipse Rich Client Platform, developers can update it to support new codes or add new tools just as easily as users can perform simulations of nuclear fuels or visualize neutron scattering data.

Full Article Here - https://www.eclipse.org/community/eclipse_newsletter/2015/january/article1.php



A collage of different visualizations tools in ICE. Clockwise from upper left: a nuclear fuel assembly, phonon data from nuclear scattering experiments, a model of nuclear plant, and a model of battery.

OpenSHMEM 1.2 Specification Released

Oscar Hernandez, Graham Lopez, Pavel Shamis, Manjunath Gorentla Venkata

OpenSHMEM specification version 1.2 was released this quarter. The specification development was ORNL led effort with the input from the participants from industry, academia, and research laboratories. Changes included in this release:

- Clear and unambiguous definition of the OpenSHMEM execution model.
- Cleaner semantics for starting and shutting down the OpenSHMEM library, which is an important requirement for tools.
- Normalization of the OpenSHMEM interfaces namespace. The prefix “shmem_” is now reserved for the OpenSHMEM interfaces in the OpenSHMEM program.
- New set of interfaces to query the version and vendor information of an OpenSHMEM implementation was introduced in this section.

This work was performed with support from ORNL, ESSC, and DoD.

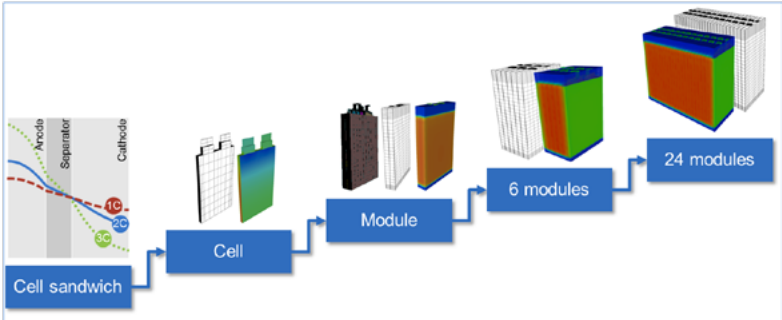
OpenSHMEM specification 1.2 is available at http://openshmem.org.

This work was performed with support from ORNL, ESSC, and DoD.

News

Battery Boost

John Turner



ORNL computing software aims to help electric vehicle industry better design high-performing and safe lithium-ion batteries through simulation.

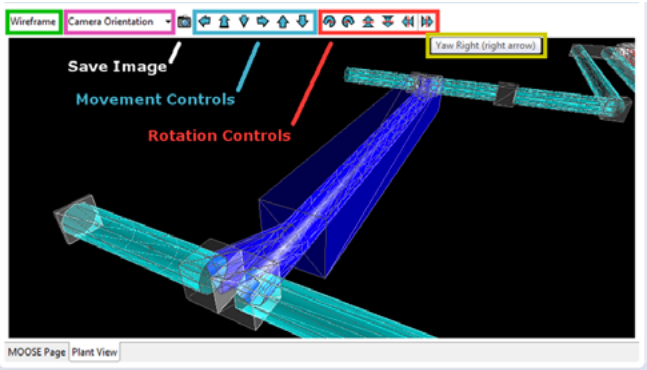
Rechargeable lithium-ion batteries are commonly found in portable electronics such as cell phones and notebook PCs. They're also gaining popularity in electric vehicles, where their compact, lightweight build and high-energy storage potential offers a more efficient and environmentally safe alternative to nickel metal hydride and lead-acid batteries traditionally used in vehicles.

Scientists at the Department of Energy's Oak Ridge National Laboratory have developed modeling software to help other researchers and battery manufacturers improve the design of lithium-ion batteries for electric vehicles. The modeling tool, known as the Virtual Integrated Battery Environment, or VIBE, will allow researchers to test lithium-ion batteries under different simulated scenarios before the batteries are built and used in electric vehicles.

Read more at: http://www.ornl.gov/ornl/news/features/2015/battery-boost

Upgrading Modeling and Simulation with the Eclipse Integrated Computational Environment

Jay Jay Billings, Alexander J. McCaskey, Andrew Bennett, Jordan H. Deyton, Hari Krishnan, Taylor Patterson, Anna Wojtowicz



Scientific Computing can be roughly divided into several different areas, one of which is that of Modeling and Simulation (M&S). Modeling and Simulation is a field that has existed, from a computing perspective, since World War II and finds its roots in government laboratories and academia. It is a field that encompasses both the art and the science of encoding the physical world into computers.

The subjects that have been investigated with computers are innumerable, with today's largest supercomputers simulating everything from cutting edge climate science to the behavior of matter at nanoscale resolution. However, while the subjects have changed and grown over the decades, many of the tools and the behaviors of the M&S community have not. A very large number of the most advanced computational studies of the physical world are done with tools that would be recognizable by a programmer from the late 1970s. The sophistication and the capability of today's software are much greater, but the tools - compilers, editors, third-party libraries, etc. - are not that different. That is to say that, on the whole, computational scientists are a command-line editing, low-level code loving kind of crowd!

The Eclipse Platform has been adopted in many different fields and, in some cases, revolutionized the state of the art. Eclipse is not used in modeling and simulation as much as it is in other areas, but it is widely known. Several years ago we asked the question, "What if the tools in Eclipse that are used forÂ authoring scientific softwareÂ could be repurposed forÂ using scientific software?" The result is the Eclipse Integrated Computational Environment (ICE); a general purpose, easily extended M&S platform that significantly updates the way computational scientists interact with their software. It improves productivity and streamlines the workflow for computational scientists when they need to create input files, launch jobs on local or remote machines, and process output. Since it is based on the Eclipse Rich Client Platform, developers can update it to support new codes or add new tools just as easily as users can perform simulations of nuclear fuels or visualize neutron scattering data.

Read more at: https://www.eclipse.org/community/eclipse_newsletter/2015/january/article1.php

News [Continued]

Local scientists map earth from inside out

David Pugmire

CSMD's David Pugmire explains how scientists at Oak Ridge National Laboratory (ORNL) are using the world's most powerful supercomputers to create a 3-D map of the Earth, and one of those supercomputers is here at ORNL.

View the interview here: http://www.wbir.com/videos/news/local/2015/03/26/local-scientists-map-earch-from-inside-out-/25224621/

Pavel Shamis' OFA talk featured on InsideHPC

Pavel Shamis

The presentation "OFA Update by ORNL," by CSMD's Pavel Shamis, is currently being featured on InsideHPC's website. According to Dr. Shamis "ORNL's supercomputing program has grown from humble beginnings to deliver some of the most powerful systems in the world. On the way, it has helped researchers deliver practical breakthroughs and new scientific knowledge in climate, materials, nuclear science, and a wide range of other disciplines."

View the entire presentation here: http://insidehpc.com/2015/03/video-ofa-update-by-ornl/

Researchers Get Warmer in Understanding High-Temperature Superconductors

Paul Kent

A group at the US Department of Energy's (DOE's) Oak Ridge National Laboratory wanted to better understand the complex interactions that enable superconductivity and needed one of the world's fastest supercomputers to help them. Using theCray XK7 Titan supercomputer at the Oak Ridge Leadership Computing Facility (OLCF), a DOE Office of Science User Facility, the team made its own leap in materials science research.

The group, led by ORNL researcher Paul Kent, advanced its understanding of superconducting by performing the first ab initio simulation of a high-temperature superconducting material, or cuprate. Read the full article [here]. https://www.olcf.ornl.gov/2015/03/10/researchers-get-warmer-in-understanding-high-temperature-superconductors/

Awards

Student's Project Wins

Rich Archibald and Melissa Yu

Melissa Yu, from Farragut High School, did her math thesis project last summer under the mentoring of Rick Archibald and Chris Symons at the Computational and Applied mathematics group last summer. Her project was focused on image registration from data obtained from experimenters at the CSNM. When images from different experimental instruments are taken of the same material, image registration is a key step to combine information from multiple sources for analysis. Melissa researched all aspects of image registration and multimodal experimental data and was able to generate a path to developing algorithms and mathematical methods to register images from different experimental devices. The ability to register multimodal data (provided by Alex Belianinov from the Institute for the Functional Imaging of Materials) will give nano scientist the capability to determine both structure and dynamics of materials. Her project won first prize in the TN Junior Science and Humanities Symposium, the Grand prize at the Southern Appalachian Science and Engineering Fair and will be going to the Intel International Science and Engineering Fair in late April. Melissa has competing offers next year for Harvard, MIT, and Princeton for next fall. She will be a HERE inter at ORNL for this coming summer.

Community Service

- David E. Bernholdt, reviewer, DOE Office of Science SBIR program
- David E. Bernholdt, reviewer, International journal of HPC Applications
- David E. Bernholdt, reviewer, Chapman & Hall publishers
- Michael J. Brim, Program Co-chair, International Workshop on the Lustre Ecosystem: Challenges and Opportunities, Annapolis, Maryland, March 3-4, 2015.
- Christian Engelmann, technical program committee member, 23rd International Heterogeneity in Computing Workshop (HCW), in conjunction with the 28th IEEE International Parallel and Distributed Processing Symposium (IPDPS) 2015, Phoenix, AZ, USA, May 19, 2015.
- Christian Engelmann, Journal on Computers & Security (COSE), peer reviewer, February, 2015.
- Christian Engelmann, technical program committee member, 3rd Workshop on Solving Problems with Uncertainties at the 15th International Conference on Computational Science (ICCS), Reykjavik, Iceland, June 1-3, 2015.

Community Service [Continued]

- Christian Engelmann, technical program committee member, 5th International Workshop on Fault-Tolerance for HPC at Extreme Scale (FTXS) at 24th International Symposium on High Performance Distributed Computing (HPDC), Portland, OR, USA, June 15-19, 2015
- Manjunath Gorentla Venkata, Programm Committee Member (Posters), 15th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing, Shenzhen, Guangdong, China, 2015
- Chung-Hsing Hsu, Program Committee Member, The 11th Workshop on High-Performance, Power-Aware Computing (HPPAC), in conjunction with the 29th IEEE International Parallel and Distributed Processing Symposium (IPDPS) 2015, Hyderabad, India, May 29, 2015.
- Christos Kartsaklis, Program Committee Member, 17th Workshop on Advances in Parallel and Distributed Computational Models (APDCM 2015)
- Christos Kartsaklis, Program Committee Member, 10th International Conference on Digital Telecommunications (ICDT 2015)
- Christos Kartsaklis, Program Committee Member, Tools for Program Development and Analysis in Computational Science Workshop, at International Conference on Computational Science (ICCS 2015)
- Christos Kartsaklis, Program Committee Member, 16th IEEE/ACIS International Conference on Software Engineering, Artificial Intelligence, Networking and Parallel/Distributed Computing (SNPD 2015)
- Christos Kartsaklis, Program Committee Member, IUPT 2015: The 5th International Symposium on Internet of Ubiquitous and Pervasive Things
- Christos Kartsaklis, Program Committee Member, INFOCOMP 2015: The 5th International Conference on Advanced Communications and Computation
- Christos Kartsaklis, Program Committee Member, 14th IEEE International Symposium on Parallel and Distributed Computing (ISPDC 2015)
- Pablo Seleson, organizer, Computational and Applied Mathematics Seminar series
- Pavel Shamis, Reviewer (Posters), 15th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing, Shenzhen, Guangdong, China, 2015
- Pavel Shamis was named co-chair of Open Fabric Alliance (OFA) Verbs Working Group
- Geoffroy Vallee, advisory board member, OCCIware project; Kick-off meeting, Jan-23, 2015
- Geoffroy Vallee, technical program committee member, 11th International Conference on Networking and Services; May 24-29, 2015, Rome, Italy
- Geoffroy Vallee, technical program committee member, 5th International Conference on Cloud Computing and Services Science; May 20-22, 2015, Lisbon, Portugal
- Guannan Zhang, Clayton Webster, Max Gunzburger, Albert Cohen, organizer, mini-symposium "High-dimensional Approximation and Integration: Analysis and Computation" SIAM Conference on Computational Science and Engineering (CSE), Salt Lake City, UT, March 14-18, 2015

Events

International Workshop on the Lustre Ecosystem: Challenges and Opportunities

The Lustre parallel file system has been widely adopted by high-performance computing (HPC) centers as an effective system for managing large-scale storage resources. Lustre achieves unprecedented aggregate performance by parallelizing I/O over file system clients and storage targets at extreme scales. Today, 7 out of 10 fastest supercomputers in the world use Lustre for high-performance storage. To date, Lustre development has

ORNL Participants:

(front row) Lora Wolfe, Neena Imam, Sarp Oral, and Feiyi Wang;

(back row) Rick Mohr, Michael Brim, Matt Ezell, Jason Hill, Corliss Thompson, and Blake Caldwell;

(absent from picture) Josh Lothian and Joel Reed.

focused on improving the performance and scalability of large-scale scientific workloads. In particular, large-scale checkpoint storage and retrieval, which is characterized by bursty I/O from coordinated parallel clients, has been the primary driver of Lustre development over the last decade. With the advent of extreme scale computing and Big

Events [Continued]

Data computing, many HPC centers are seeing increased user interest in running diverse workloads that place new demands on Lustre.

In early March, the International Workshop on the Lustre Ecosystem: Challenges and Opportunities was held in Annapolis, Maryland at the Historic Inns of Annapolis Governor Calvert House. This workshop series is intended to help explore improvements in the performance and flexibility of Lustre for supporting diverse application workloads. This year's workshop was the inaugural edition, and the goal was to initiate a discussion on the open challenges associated with enhancing Lustre for diverse applications, the technological advances necessary, and the associated impacts to the Lustre ecosystem. The workshop program featured a day of tutorials and a day of technical paper presentations.

The workshop kicked off on March 3rd with a keynote speech from Eric Barton, Lead Architect of the High Performance Data Division at Intel. The keynote, titled "From Lab to Enterprise - Growing the Lustre Ecosystem", provided a great starting point for the workshop by identifying current pitfalls in moving Lustre into new application domains with potentially conflicting demands compared with traditional HPC scientific applications, and highlighting Intel's ongoing efforts to enhance Lustre's core feature set and subsystems in support of these new diverse workloads.

After the keynote, experts from the Oak Ridge Leadership Computing Facility (OLCF) at ORNL gave tutorials on the best practices used and lessons learned in deploying and operating one of the world's largest center-wide Lustre installations. OLCF tutorial presenters included Blake Caldwell, Matt Ezell, Jason Hill, Sarp Oral, and Feiyi Wang. The first day concluded with an "Ask the OLCF" discussion panel where workshop attendees had the opportunity to ask the tutorial presenters additional questions related to Lustre administration and monitoring.

On March 4th, a collection of international speakers from academia, industry, and national laboratories gave technical presentations in four sessions. The first session focused on characterizing and enhancing Lustre's functionality and performance in support of diverse workloads. The second session highlighted recent advances in managing large-scale Lustre installations. The third session introduced new efforts to monitor large-scale Luste installations using holistic techniques that combine information from a wide variety of sources. The final session covered advancements in storage architectures and technologies aimed at improving the Lustre's reliability and performance.

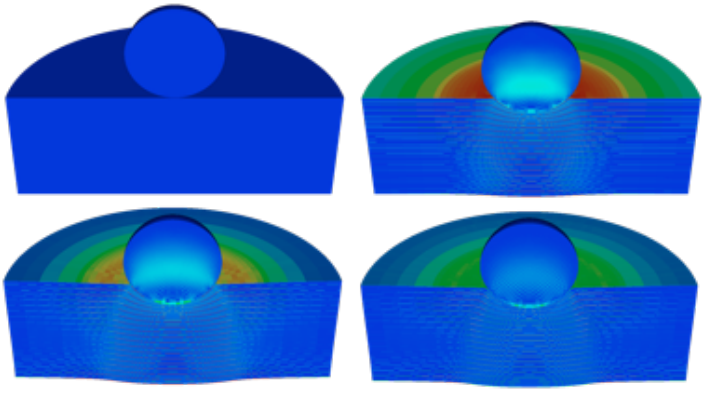
Presentation content for the keynote, tutorials, and technical presentations can be found at http://lustre.ornl.gov/ecosystem/agenda.html.

The workshop was organized by ORNL and sponsored by the DoD-HPC Research Program at ORNL. The workshop program co-chairs were Neena Imam, Michael Brim, and Sarp Oral. Jason Hill served as the tutorials chair.

Li-ion Battery Safety Modeling Presentation

Srikanth Allu, Sergiy Kalnaus, Abhishek Kumar, Sreekanth Pannala, Srdjan Simunovic, Hsin Wang

On Jan. 23, 2015, Computational Engineering and Energy Science Group Leader John A. Turner presented work of the ORNL battery simulation team at the Society of Automotive Engineers (SAE) 2015 Government/Industry Meeting in Washington, DC, in a presentation titled "Li-ion Battery Safety Modeling" in a session organized by Phil Gorney of DOT/NHTSA.



Spherical indenter crushing a Li-ion pouch cell battery made up of multiple component layers.

We report results of an on-going computational and experimental effort supported by DOT/NHTSA to simulate a battery's electrochemical, thermal, and structural responses under mechanical impact conditions. The characteristic failure features require micrometer resolution for typical cell components, which span centimeters. Under the DOE/EERE Computer Aided Engineering for Batteries (CAEBAT) project, ORNL has developed the Virtual Integrated Battery Environment (VIBE), a transient coupled-physics simulation environment for batteries, with emphasis on Li-ion. VIBE has been extended to couple impact mechanics and its interaction with other physics components. The model is being used to analyze and correlate with existing mechanical test data from ORNL and others. New tests for both cells and cell stacks are being developed and conducted by ORNL to support model development.

CSMD Seminar Series

- March 31, 2015 - Keita Teranishi : Local Failure Local Recovery for large scale SPMD applications
- March 30, 2015 - Sarah Osborn : Solutions Strategies for Stochastic Galerkin Discretizations of PDEs with

Events [Continued]

Random Data

- March 30, 2015 - Emil Alexov : Revealing the molecular mechanism of Snyder-Robinson Syndrome and rescuing it with small molecule binding
- March 9, 2015 - Mark Kim: GPU-enabled Particle Systems for Visualization
- March 6, 2015 - Sungahn Ko: Aided decision-making through visual analytics systems for big data
- February 3, 2015 - Sergiy Kalnaus: Predictive modeling for electrochemical energy storage
- January 29, 2015 - Deepak Majeti: Portable Programming Models for Heterogeneous Platforms
- January 6, 2015 - David M. Weiss: Industrial Strength Software Measurement

CAM Seminar Series

- January 13, 2015 - Dr. Zhiwen Zhang : Multiscale Model Reduction for Stochastic Partial Differential Equations
- January 15, 2015 - Dr. Ke Shi : Multiscale Hybridizable DG methods for Flows in Porous Media
- January 20, 2015 - Dr. Lin Mu : Applications of Weak Galerkin Finite Element Methods
- January 22, 2015 - Dr. Masayuki Yano : Towards Reliable and Automated Simulations in Continuum Mechanics
- January 29, 2015 - Dr. Yehuda Braiman : Transitions from Oscillatory to Smooth Fracture Propagation in Viscoelastic Materials
- February 3, 2015 - Mr. David Witman : Using Reduced Order Modeling to Solve Nonlocal and Anomalous Diffusion Problems
- February 3, 2015 - Mr. Lukas Bystricky : Modeling Carbon Nanotubes in Injection Molding
- February 12, 2015 - Dr. Feng Bao : Numerical Algorithms for Nonlinear Filtering Problems
- February 27, 2015 - Dr. Jichun Li : Finite Element Analysis and Modeling of Invisibility Cloaks with Metamaterials
- March 5, 2015 - Dr. Richard Barnard : Sensitivity Analysis in Radiotherapy Dose Calculations and Bilevel Optimization for Parameter Identification
- March 19, 2015 - Dr. Eirik Endeve : Bound-Preserving Discontinuous Galerkin Methods for Conservative Phase Space Advection
- March 26, 2015 - Dr. Garrett Granroth : Mathematical and Computational Challenges in Neutron Scattering

ASCR Workshop on Quantum Computing for Science (February 17-18, 2015)

Travis Humble

At the request of the Department of Energy's (DOE) Office of Advanced Scientific Computing Research (ASCR), this program committee has been tasked with organizing a workshop to assess the viability of quantum computing technologies to meet the computational requirements in support of DOE's science and energy mission and to identify the potential impact of these technologies. As part of the process, the program committee is soliciting community input in the form of position papers. The program committee will review these position papers and, based on the fit of their area of expertise and interest, selected contributors will have the opportunity to participate in the workshop currently planned for February 17-18th, 2015 in Bethesda, MD.

Visit the site [here].

Upcoming Events

Advances in Scientific Computing and Applied Mathematics (October 9-12)

Clayton Webster

The conference on "Advances in scientific computing and applied mathematics" will take place October 9-12 in the Stratosphere Hotel in Las Vegas, Nevada. The conference is co-sponsored by the Oak Ridge National Laboratory, Sandia National Laboratories and The Office of Science, Advanced Simulation Research Computing (ASCR), at the Department of Energy.

We also invite the participants to submit an original research paper to a special issue of the journal "Computers and Mathematics with Applications" to honor Prof. Max Gunzburger's 70th birthday. The issue will be edited by Drs. Pavel Bochev, Qiang Du, Steven L. Hou and Clayton Webster. The submissions are due by March 31st, 2015. We look forward to your contribution.

Visit site [here].

OpenSHMEM 2015: Second workshop on OpenSHMEM and Related Technologies (August 4-6)

Pavel Shamis

The OpenSHMEM workshop is an annual event dedicated to the promotion and advancement of the OpenSHMEM programming interface and to helping shape its future direction. It is the premier venue to discuss and present the latest developments, implementation technologies,

Upcoming Events [Continued]

tools, trends, recent research ideas and results related to OpenSHMEM. This year's workshop will explore the ongoing evolution of OpenSHMEM as a next generation PGAS programming model to address the needs of exascale applications. The focus will be on future extensions to improve OpenSHMEM on current and upcoming architectures. Although, this is an OpenSHMEM specific workshop, we welcome ideas used for other PGAS languages/APIs that may be applicable to OpenSHMEM.

Visit site [here].

Beyond Lithium Ion VIII (June 2-4)

Sreekanth Pannala and Jason Zhang

Significant advances in electrical energy storage could revolutionize the energy landscape. For example, widespread adoption of electric vehicles could greatly reduce dependence on finite petroleum resources, reduce carbon dioxide emissions and provide new scenarios for grid operation. Although electric vehicles with advanced lithium ion batteries have been introduced, further breakthroughs in scalable energy storage, beyond current state-of-the-art lithium ion batteries, are necessary before the full benefits of vehicle electrification can be realized.

Motivated by these societal needs and by the tremendous potential for materials science and engineering to provide necessary advances, a consortium comprising IBM Research and five U.S. Department of Energy National Laboratories (National Renewable, Argonne, Lawrence Berkeley, Pacific Northwest, and Oak Ridge) will host a symposium June 2-4, 2015, at Oak Ridge National Laboratory. This is the eighth in a series of conferences that began in 2009.

Visit site [here].

Numerical and Computational Developments to Advance Multiscale Earth System Models (MSESM) (June 1-3)

Kate Evans

Substantial recent development of Earth system models has enabled simulations that capture climate change and variability at ever finer spatial and temporal scales. In this workshop we seek to showcase recent progress on the computational development needed to address the new complexities of climate models and their multi-scale behavior to maximize efficiency and accuracy. This workshop brings together computational and domain Earth scientists to focus on Earth system models at the largest scales for deployment on the largest computing and data centers.

Topics include, but are not limited to:

- multi-scale time integration
- advection schemes
- regionally- and dynamically-refined meshes
- many-core acceleration techniques
- examination of multi-scale atmospheric events
- coupled interactions between model components (such as atmosphere, ocean, and land), and techniques to make these couplings computationally tractable

Visit the site [here].

Publications

Abstract - Conference

Braiman, Yehuda (ORNL), Neschke, Brendan (ORNL), Barhen, Jacob (ORNL); *Reduced Order Model for Fractue Propagation in Viscoelastic Materials for High Speed Propagation and Subject to Strong Nonlocal Resistance Force*

Rastogi, Deeksha (ORNL), Mei, Rui (ORNL), Ashfaq, Moetasim (ORNL); *Climate Extremes in a High-Resolution Regional Model Ensemble over the Continental United States*, 1/2015

Turner, John A. (ORNL), Allu, Srikanth (ORNL), Berrill, Mark A. (ORNL), Elwasif, Wael R. (ORNL), Kalnaus, Sergiy (ORNL), Kumar, Abhishek (ORNL), Lebrun-Grandie, Damien T. (ORNL), Pannala, Sreekanth (ORNL), Simunovic, Srdjan (ORNL); *Safer Batteries through Coupled Multiscale Modeling*, 6/2015

Turner, John A. (ORNL), Babu, Sudarsanam Suresh (ORNL), Pannala, Sreekanth (ORNL); *Modeling and Simulation for Additive Manufacturing: An Integrated Approach*, 2/2015

Journal Article

Ahn, Tae-Hyuk (ORNL), Chai, JJ (ORNL), Pan, Chongle (ORNL); *Sigma: Strain-level inference of genomes from metagenomic analysis for biosurveillance*, Bioinformatics, pp. 177-177, 1/2015

Archibald, Richard K. (ORNL), Evans, Katherine J. (ORNL), Salinger, Andrew G. (Sandia National Laboratories (SNL)); *Accelerating Time Integration for Climate Modeling Using GPUs*, Procedia Computer Science, 1/2015

Cao, Zhen (University of Connecticut, Storrs), Stevens, Mark J. (Sandia National Laboratories (SNL)), Carrillo, Jan-Michael Y. (ORNL), Dobrynin, Andrey (University of Connecticut, Storrs); *Adhesion and Wetting of Soft Nanoparticles on Textured Surfaces: Transition between Wenzel and Cassie-Baxter States*, Langmuir, 1/2015

Publications [Continued]

Endeve, E., Hauck, C.D., Xing, Y., Mezzacappa, A., *Bound-Preserving Discontinuous Galerkin Methods for Conservative Phase Space Advection in Curvilinear Coordinates*, Journal of Computational Physics, 287, 151-183, 2015

Kennedy, Joseph H. (ORNL), Pettit, Dr. Erin C (University of Alaska, Fairbanks); *The response of fabric variations to simple shear and migration recrystallization*, Journal of Glaciology

Kumar, Rajeev (ORNL), Kilbey, II, S Michael (ORNL), Ankner, John Francis (ORNL), Heller, William T. (ORNL), Chen, Jihua (ORNL), Sides, Scott (ORNL), Browning, Jim (ORNL), Lokitz, Bradley S. (ORNL), Sumpter, Bobby G. (ORNL); *Microphase separation in thin films of lamellar forming poydisperse di-block copolymers*, RSC Advances, 2/2015

Liu, Bo (ORNL), Tong, Xin Tony (ORNL), Robertson, Lee (ORNL), Jiang, Chenyang Peter (ORNL), Brown, Daniel R. (ORNL); *Development of stable, narrow spectral line-width, fiber delivered laser source for spin exchange optical pumping*, Applied Optics

Mittal, Sparsh (ORNL), Vetter, Jeffrey S. (ORNL); *EqualWrites: Reducing Intra-set Write Variations for Enhancing Lifetime of Non-volatile Caches*, IEEE Transactions on VLSI Systems, 2015

Parham, Paul (University of Liverpool), Waldock, Johanna (Imperial College, London), Christophides, George (Imperial College, London), Hemming, Deborah (Met Office Hadley Centre), Agusto, Folashade (Austin Peay State University), Evans, Katherine J. (ORNL), Fefferman, Nina (Rutgers University), Gaff, Holly (Old Dominion University), Gumel, Abba (Arizona State University), LaDeau, Shannon (The University of Tennessee), Lenhart, Suzanne (University of Tennessee, Knoxville (UTK)), Mickens, Ronald (Clark Atlanta University), Naumova, Elena (Tufts University), Ostfeld, Richard (Cary Institute of Ecosystem Studies, New York), Ready, Paul (Natural History Museum), Thomas, Matthew (Pennsylvania State University), Velasco-Hernandez, Jorge (Universidad Nacional Autonoma de Mexico (UNAM)), Edwin, Michael (University of Notre Dame, IN); *Climate, Environmental, and Socioeconomic Change - Weighing up the Balance in Vector-Borne Disease Transmission*, Philosophical Transactions of the Royal Society B, 4/2015

Paugh, Steven W (St. Jude Children's Research Hospital), Coss, David R (St. Jude Children's Research Hospital), Laudermilk, Lucas T (St. Jude Children's Research Hospital), Ferreira, Antonio M (St. Jude Children's Research Hospital), Waddell, M Brett (St. Jude Children's Research Hospital), Ridout, Granger (St. Jude Children's Research Hospital), Naeve, Deanna (St. Jude Children's Research Hospital), Leuze, Michael Rex (ORNL), LoCascio, Philip F (University of Oxford), Panetta, John C (St. Jude Children's Research Hospital), Wilkinson, Mark R (St. Jude Children's Research Hospital), Pui, Ching-Hon (St. Jude Children's Research Hospital), Naeve, Clayton W (St. Jude Children's Research Hospital), Uberbacher, Edward C. (ORNL), Evans, William E (St. Jude Children's Research Hospital); *MicroRNAs form triplexes with double stranded DNA at specific DNA sequences; a new mechanism via which microRNAs can directly alter gene expression*, PLoS Computational Biology

Philip, Bobby (ORNL), Berrill, Mark A. (ORNL), Allu, Srikanth (ORNL), Hamilton, Steven P. (ORNL), Sampath, Rahul S. (ORNL), Clarno, Kevin T. (ORNL), Dilts, Gary (Los Alamos National Laboratory (LANL)); *A Parallel Multi-Domain Solution Methodology Applied to Nonlinear Thermal Transport Problems in Nuclear Fuel Pins*, Journal of Computational Physics, pp. 171-171, 4/2015

Radhakrishnan, Balasubramaniam (ORNL), Nicholson, Don M. (ORNL), Eisenbach, Markus (ORNL), Ludtka, Gerard Michael (ORNL), Vlassiouk, Ivan V. (ORNL), Rios, Orlando (ORNL); *Magnetic Field Induced Alignment of a Fe Nanoparticle above the Curie Temperature*, Scripta Materialia

Reshniak, V., Khaliq, A., Voss D., Zhang, G., Split-step Milstein methods for multi-channel stiff stochastic differential systems, Applied Numerical Mathematics, 89 (2015), pp. 1-23.

Woltornist, Steven (University of Connecticut, Storrs), Carrillo, Jan-Michael Y. (ORNL), Xu, Thomas (University of Connecticut, Storrs), Dobrynin, Andrey (University of Connecticut, Storrs), Adamson, Douglas (University of Connecticut, Storrs); *Polymer/Pristine Graphene Based Composites: From Emulsions to Strong, Electrically Conducting Foams*, Macromolecules, 1/2015

Zhang, G., Webster, C., Gunzburger, M., Burkardt, J., A hyper-spherical adaptive sparse-grid method for high-dimensional discontinuity detection, SIAM Journal of Numerical Analysis, to appear in 2015.

ORNL Report

Endeve, Eirik (ORNL), Hauck, Cory D. (ORNL), Xing, Yulong (ORNL), Mezzacappa, Anthony (ORNL); *Bound-Preserving Discontinuous Galerkin Methods for Conservative Phase Space Advection in Curvilinear Coordinates*

Endeve, Eirik (ORNL), Hauck, Cory D. (ORNL), Xing, Yulong (ORNL), Mezzacappa, Anthony (ORNL); *Towards Robust Discontinuous Galerkin Methods for General Relativistic Neutrino Radiation Transport*

McCaskey, Alex (ORNL), Wojtowicz, Anna (ORNL), Deyton, Jordan H. (ORNL), Patterson, Taylor C. (ORNL), Billings, Jay Jay (ORNL); *An Update on Improvements to NiCE Support for RELAP-7*, 1/2015

Seleson, P., Parks, M. L., *Links between Peridynamic and Atomistic Models*, Tech. Rep. ORNL/TM-2015/108, Oak Ridge National Laboratory, March 2015.

Publications [Continued]

Other

Patterson, Taylor C. (ORNL), Deyton, Jordan H. (ORNL), Wojtowicz, Anna (ORNL), Bennett, Andrew R. (ORNL), Krishnan, Harinarayan (Lawrence Berkeley National Laboratory (LBNL)), McCaskey, Alex (ORNL), Billings, Jay Jay (ORNL); *Eclipse ICE: A Cool Approach to Modeling and Simulation*, 3/2015

Polcari, John J. (ORNL); An Informative Interpretation of Decision Theory: *Scalar Performance Measures for Binary Decisions*, 1/2015

Paper in Conference Proceedings

Archibald, Evans, Salanger, *Accelerating Time Integration for Climate Modeling Using GPUs*, Journal of Computational Science, in press.

Belianinov, Vasudevan, Strelcov, Steed, Yang, Tselev, Jesse, Biegalski, Shipman, Symons, Borisevich, Archibald, and Kalinin, *Big Data and Deep Data in Scanning and Electron Microscopies: Functionality from Multidimensional Data Sets*, Advanced Structural and Chemical Imaging, in press

Brim, Michael J. (ORNL), Lothian, Josh (ORNL); *Monitoring Extreme-scale Lustre Toolkit*, International Workshop on The Lustre Ecosystem: Challenges and Opportunities

Collins, William D (Lawrence Berkeley National Laboratory (LBNL)), Johansen, Hans (Lawrence Berkeley National Laboratory (LBNL)), Evans, Katherine J. (ORNL), Woodward, Carol S. (Lawrence Livermore National Laboratory (LLNL)), Caldwell, Peter (Lawrence Livermore National Laboratory (LLNL)); *Progress in Fast, Accurate Multi-scale Climate Simulations*, International Conference on Computational Science

Engelmann, Christian (ORNL), Naughton, III, Thomas J. (ORNL); *A Network Contention Model for the Extreme-scale Simulator*, 34th IASTED International Conference on Modelling, Identification and Control (MIC) 2015, 2/2015

Gardner, David (Lawrence Livermore National Laboratory (LLNL)), Woodward, Carol S. (Lawrence Livermore National Laboratory (LLNL)), Evans, Katherine J. (ORNL); *On the Use of Finite Difference Matrix-Vector Products in Newton-Krylov Solvers for Implicit Climate Dynamics with Spectral Elements*, Procedia Computer Science, International Conference on Computational Science

Gunzburger, M., Webster C., Zhang, G., Sparse collocation methods for stochastic interpolation and quadrature, Handbook of Uncertainty Quantification, Springer, 2015.

Kim, Jungwon (ORNL), Lee, Seyong (ORNL), Vetter, Jeffrey S. (ORNL); *An OpenACC-Based Unified Programming Model for Multi-accelerator Systems*, ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming, pp. 258-258, 2/2015

Radhakrishnan, Balasubramaniam (ORNL), Gorti, Sarma B. (ORNL), Babu, Sudarsanam Suresh (ORNL); *LARGE SCALE PHASE FIELD SIMULATIONS OF MICROSTRUCTURE EVOLUTION DURING THERMAL CYCLING OF TI-6AL-4V*, International Conference on Solid-Solid Phase Transformations in Inorganic Materials (PTM)

Sen, Satyabrata (ORNL), Barhen, Jacob (ORNL); *Adaptive OFDM Waveform Design for Spatio-Temporal-Sparsity Exploited STAP Radar*, SPIE Defense and Security Symposium, Radar Sensor Technology XIX Conference

Slattery, Stuart R. (ORNL), Hamilton, Steven P. (ORNL), Evans, Thomas M. (ORNL); *A Modified Moving Least Square Algorithm for Solution Transfer on a Spacer Grid Surface*, ANS MC2015 - Joint International Conference on Mathematics and Computation, Supercomputing in Nuclear Applications and the Monte Carlo Method

Toth, Alex (North Carolina State University), Kelley, C. T. (North Carolina State University), Slattery, Stuart R. (ORNL), Hamilton, Steven P. (ORNL), Clarno, Kevin T. (ORNL), Pawlowski, R. P. P. (Sandia National Laboratories (SNL)); *Analysis of Anderson Acceleration on a Simplified Neutronics/Thermal Hydraulics System*, NS MC2015 - Joint International Conference on Mathematics and Computation (M&C), Supercomputing in Nuclear Applications (SNA) and the Monte Carlo (MC) Method, 4/2015

Wasserman, Archibald, and Gelb, "Image Reconstruction from Fourier Data Using Sparsity of Edges Polynomial Annihilation Sparsifying Transform", Journal of Scientific Computing, 2014.

Wayne, Archibald, et. al., "Accelerated Application Development: The ORNL Titan Experience", Computers & Electrical Engineering, in press

Presentation Material - Conference

Archibald, R., Hauck, C., Multivariate Polynomial Interpolation and Annihilation The Connection to Gaussian Processes SIAM Conference on Computational Science and Engineering (CSE), Salt Lake City, UT, March 14-18, 2015

Bao, Feng, Cao, Yanzhao, Webster, Clayton, Zhang, Guannan, *A meshfree implicit filter algorithm for solving nonlinear filtering problems*, SIAM South-East Atlantic Annual Meeting SEAS 2015, University of Alabama at Birmingham, March 21-22, 2015.

Bao, Feng, *Numerical algorithms for nonlinear filtering problems*, ORNL CAM seminar talk, University of Tennessee stochastic seminar talk and SIAM CSE 15, Salt Lake City, UT

Bernholdt, David E. (ORNL), Elwasif, Wael R. (ORNL), Foley, Samantha S. (ORNL), Batchelor, Donald B. (ORNL); *Software Productivity Application: Integrated Modeling for Fusion Energy*, SIAM Conference on Computational Science and Engineering (SIAM CSE) 2015

Bernholdt, David E. (ORNL), Elwasif, Wael R. (ORNL), Foley, Samantha S. (ORNL); *Workflow Support for Integrated Modeling for Fusion Energy*, SOS19: Better, Faster, Cheaper,

Publications [Continued]

Pick Two

Crockat, Michael, Garrett, C. Kristopher, *A High Order, Implicit, Hybrid Solver for Linear Kinetic Equations*, SIAM Conference on Computational Science and Engineering (CSE), Salt Lake City, UT, March 14-18, 2015

Dexter, Nick, *The Computational Complexity of Stochastic Galerkin and Collocation Methods for PDEs with Random Coefficients*, SIAM Conference on Computational Science and Engineering (CSE), Salt Lake City, UT, March 14-18, 2015

Endeve, E., *Bound-Preserving Discontinuous Galerkin Methods for Conservative Phase Space Advection*,Computational and Applied Mathematics Seminar, Oak Ridge National Laboratory, March 19, 2015

Endeve, E., *Solving Kinetic Equations to Model the Core-Collapse Supernova Explosion Mechanism*, Invited talk given at the mini-symposium Computational Methods for Kinetic Equations and Related Models, at the SIAM CSE 2015 conference in Salt Lake City, Utah, March 15, 2015

Fann, G., *Adaptive multiresolution 3D Hartree-Fock-Bogoliubov solver for nuclear structure, International Workshop on New Frontier of Numerical Methods for Many-Body Correlations — Methodologies and Algorithms for Fermion Many-Body Problems*, University of Tokyo, March 22, 2015

Garrett, C. Kristopher, Hauck, Cory, *An Implicit Hybrid Solver for Kinetic Semiconductor Equations*, SIAM Conference on Computational Science and Engineering (CSE), Salt Lake City, UT, March 14-18, 2015

Jantsch, Peter, Galindo, Diego, Webster, Clayton, Zhang, Guannan, *Accelerating Stochastic Collocation Methods for Random PDEs,* SIAM Conference on Computational Science and Engineering (CSE), Salt Lake City, UT, March 14-18, 2015

Kim, Jungwon (ORNL), Lee, Seyong (ORNL), Vetter, Jeffrey S. (ORNL); *PMAS: A Unified Programming Model for Multi-Accelerator Systems*, GPU Technology Conference

Lu, Dan (ORNL), Gunzburger, Max D. (ORNL), Webster, Clayton G. (ORNL), Barbier, Charlotte N. (ORNL); *A multilevel Monte Carlo approach for predicting the uncertainty in oil reservoir simulations*, AGU fall meeting

McCaskey, Alex (ORNL), Patterson, Taylor C. (ORNL), Billings, Jay Jay (ORNL); *Modernizing Simulation Input Generation and Post-Simulation Data Visualization with Eclipse ICE*, EclipseCon North America 2015

Seleson, P., *A Concurrent Multiscale Blending Scheme for Local/Nonlocal Coupling*, AMS Spring Southeastern Sectional Meeting, University of Alabama in Huntsville, March 27-29, 2015, Huntsville, AL

Stoyanov, M., Webster, C., *Analysis of Krylov Solver Resilience in the Presence of Soft-Faults*, SIAM Conference on Computational Science and Engineering (CSE), Salt Lake City, UT, March 14-18, 2015

Tran, H., DeVore, R., Webster, C., Zhang, G., *Quasi-optimal polynomial approximations for parameterized PDEs with deterministic and stochastic coefficients*, Comp Math Seminar, Clemson University, March 2015.

Tran, H., DeVore, R., Webster, C., Zhang, G., *Quasi-optimal polynomial approximations for parameterized PDEs with deterministic and stochastic coefficients*, SIAM South-East Atlantic Annual Meeting SEAS 2015, University of Alabama at Birmingham, March 21-22, 2015.

Turner, John A. (ORNL), Allu, Srikanth (ORNL), Elwasif, Wael R. (ORNL), Kalnaus, Sergiy (ORNL), Kumar, Abhishek (ORNL), Pannala, Sreekanth (ORNL), Simunovic, Srdjan (ORNL), Wang, Hsin (ORNL); *Advanced Crash Testing and Simulations for Automotive Batteries*, 32nd International Battery Conference & Symposium

Turner, John A. (ORNL), Allu, Srikanth (ORNL), Kalnaus, Sergiy (ORNL), Kumar, Abhishek (ORNL), Pannala, Sreekanth (ORNL), Simunovic, Srdjan (ORNL), Wang, Hsin (ORNL); *Li-ion Battery Safety Modeling*, Society of Automotive Engineers 2015 Government/Industry Meeting

Turner, John A. (ORNL); *SOS20 announcement at SOS19*, SOS19

Zhang, G., *A Stochastic Approach for a Class of Anomalous Diffusion Problems*, The 9th International Conference on Computational Physics, Singapore

Zhang, G., *Reduced-basis methods for a class of nonlocal diffusion equations with random input data*, SIAM Conference on Computational Science and Engineering (CSE), Salt Lake City, UT, March 14-18, 2015

Presentation Material - No Conference

Brim, Michael J. (ORNL); *The Evolution of Scalable Shared Storage*

Lingerfelt, Eric J. (ORNL); *Accelerating Scientific Discovery with the Bellerophon Software System*

Roth, Philip C. (ORNL), *Meredith, Jeremy S. (ORNL); Plasma Surface Interactions: EAVL Update*

Roth, Philip C. (ORNL); *Plasma Surface Interactions: XOLOTL Performance Activities*

Turner, John A. (ORNL); *Multi-Institutional Development of Scientific Software: Lessons Learned in CASL*

Turner, John A. (ORNL); *Multi-Institutional Development of Scientific Software: Lessons Learned in CASL*

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 nine Groups. These Groups and their Group Leaders are:

- Complex Systems – Jacob Barhen
- Computational Biomolecular Modeling & Bioinformatics – Mike Leuze
- Computational Chemical and Materials Sciences – Bobby Sumpter
- Computational Earth Sciences – Kate Evans
- Computational Engineering and Energy Sciences – John Turner
- Computational Applied 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

CONTACTS

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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