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CSMD

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Events

6th Workshop on Resiliency in High Performance Computing (Resilience)
2013 Christian Engelmann, program chair

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

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

Highlights

Using Performance Tools to Support Experiments in (HPC) Resilience

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

The high performance computing (HPC) community is working to address concerns associated with fault tolerance and resilience in current and future large scale computing platforms. This is driving enhancements in the programming environments, specifically research on enhancing message passing interface (MPI) to support fault tolerant computing capabilities. As these enhancements emerge, tools for resilience experimentation are becoming more important. In the workshop paper titled, "Using Performance Tools to Support Experiments in HPC Resilience," we consider how HPC performance-focused tools and methods can be extended ("repurposed") to benefit the resilience community.

The paper describes the initial motivation to leverage standard HPC performance analysis techniques to aid in developing diagnostic tools to assist fault tolerance experiments for HPC applications. These diagnostic procedures help to provide context for the system when the errors (failures) occurred. We describe the extension of an existing MPI tracing package (i.e., DUMPI) to support the User Level Failure Mitigation (ULFM) specification that has been proposed to the MPI Forum by the Fault Tolerance Working Group (MPI-FTWG). The data obtained from these traces can assist application developers and FT implementers for diagnosing problems and help with postmortem analysis. To investigate the usefulness of the trace tool we extended a simple molecular dynamics application to use the ULFM enhancements to MPI. Our initial experiments used the trace files from the tests to help gain insights into the context of the job during resilience experiments. The traces helped to highlight two problems we encountered during fault injection experiments: i) a fault-injection logic error that resulted in correct results (application output), but more ranks than anticipated being killed; ii) an issue in failure detection/propagation with the ULFM prototype that was effected by the method used to simulate the rank failure. The trace files also help to explain changes to overall performance when MPI fault tolerance mechanisms are employed.

"Using Performance Tools to Support Experiments in HPC Resilience," Thomas Naughton, Swen Böhm, Christian Engelmann and Geoffroy Vallée," (To appear) Lecture Notes in Computer Science: Proceedings of the 19th European Conference on Parallel and Distributed Computing (Euro-Par) Workshops: 6th Workshop on Resiliency in High Performance Computing (Resilience) in Clusters, Clouds, and Grids, August 26, 2013, Aachen, Germany. Springer Verlag, Berlin, Germany.

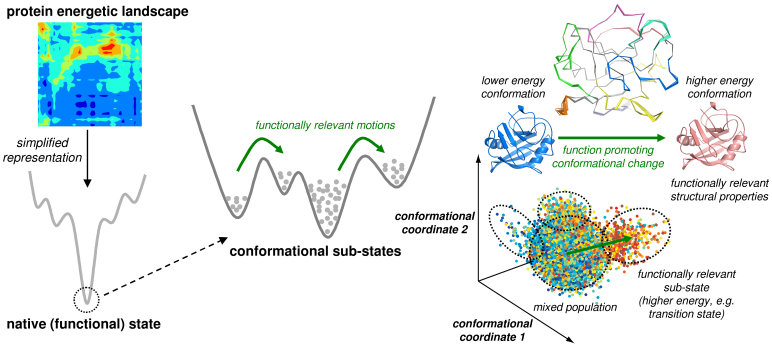
OAK RIDGE National Laboratory

Highlights (continued)

Conformational Diversity and Sub-states in Enzyme Catalysis

ORNL Team Member: Pratul Agarwal

Enzymes are great biocatalysts, and have attracted significant interest for industrial applications (including cellulosic ethanol) due to their remarkable catalytic efficiencies. The understanding of factors that enable enzymes to achieve the high catalytic efficiency will have large impact through design of new and powerful biocatalysts. Unfortunately, the understanding of these factors has largely remained a mystery. Using joint computational-experimental methodology, we have developed a unique technique named quasi-anharmonic analysis (QAA) for identification of conformational diversity and conformational sub-states associated with enzyme function. As a result of this approach, we have been able to develop a novel enzyme engineering approach that shows ~3000% increase in enzyme activity. [more]



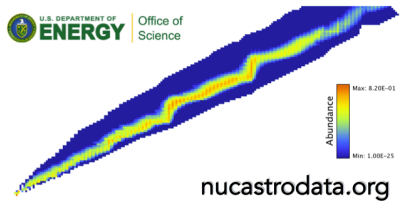
Spin-Resolved Self-Doping Tunes The Intrinsic Half-Metallicity Of AlN Nanoribbons

ORNL Team Members: Alejandro Lopez-Bezanilla, P. Ganesh, Paul R. C. Kent, and Bobby G. Sumpter

A first-principles theoretical study of electric field- and strain-controlled intrinsic half-metallic properties of zigzagged aluminium nitride (AlN) nanoribbons reveals that the half-metallic property of AlN ribbons can undergo a metallic or semiconducting transition with application of an electric field or uniaxial strain. An external transverse electric field induces full charge screening, rendering the material semiconducting, while an uniaxial strain, varying from compressive to tensile, causes the spin-resolved selective self-doping to increase the half-metallic character of the ribbons. The relevant strain-induced changes in electronic properties arise from band structure modifications at the Fermi level as a consequence of a spin-polarized charge transfer between p-orbitals of the N and Al edge atoms in a spin-resolved self-doping process. The band structure tunability indicates the possibility of rationally designing magnetic nanoribbons with tunable electronic structure by deriving edge states from elements with sufficiently different localization properties. [more]

Simulating Element Creation in Supernovae with the Computational Infrastructure for Nuclear Astrophysics at nucastrodata.org

ORNL Team Members: Eric Lingerfelt, Michael Smith (PI), W. Raphael Hix, and Chris Smith



The elements, which make up our bodies and the world around us, are produced in violent stellar explosions. Computational simulations of the element creation processes occurring in these cataclysmic phenomena are complex calculations that track the abundances of thousands of species of subatomic nuclei that are interrelated by ~60,000 thermonuclear reaction rates stored in continually updated databases. Previously, delays of up to a decade were experienced before the latest experimental reaction rates were used in astrophysical simulations. The Computational Infrastructure for Nuclear Astrophysics (CINA), freely available at the website nucastrodata.org, reduces this delay from years to minutes! With over 100 unique software tools developed over the last decade, CINA comprises a “lab-to-star” connection. It is the only cloud computing software system in this field and it is accessible via an easy-to-use, web-deliverable, cross-platform Java application. Currently, CINA has registered users from over 32 countries and 141 institutions with new users added every week. [more]

This work is funded by the DOE’s Office of Nuclear Physics under the US Nuclear Data Program.

Tools for Simulation and Benchmark Generation at Exascale

ORNL Team Member: Christian Engelmann with Mahesh Lagadapati (NCSU), and Frank Mueller (NCSU)

The path to exascale high-performance computing (HPC) poses several challenges related to power, performance, resilience, productivity, programmability, data movement, and data management. Investigating the performance of parallel applications at scale on future architectures and the performance impact of different architecture choices is an important component of HPC hardware/software co-design. Simulations using models of future HPC systems and communication traces from applications running on existing HPC systems can offer an insight into the performance of future architectures. This work targets technology developed for scalable application tracing of communication events and

memory profiles, but can be extended to other areas, such as I/O, control flow, and data flow. It further focuses on extreme-scale simulation of millions of Message Passing Interface (MPI) ranks using a lightweight parallel discrete event simulation (PDES) toolkit for performance evaluation. Instead of simply replaying a trace within a simulation, the approach is to generate a benchmark from it and to run this benchmark within a simulation using models to reflect the performance characteristics of future-generation HPC systems. This provides a number of benefits, such as eliminating the data intensive trace replay and enabling simulations at different scales. A recent accomplishment utilizes the ScalaTrace tool from North Carolina State University (NCSU) to generate scalable trace files, the ScalaBenchGen tool from NCSU to generate the benchmark, and ORNL's extreme-scale simulator, xSim, tool to run the benchmark within a simulation. Early results show that Execution times of both the original application and the generated benchmarks are similar for the FT benchmark from the NAS parallel benchmark suite. The mean error rate is only 5% for FT, while a rate of 20% is observed for the IS benchmark from the NAS parallel benchmark suite. Ongoing work focuses on handling more benchmarks during the generation process and on improving accuracy.

Read the supporting document [**HERE**].

Optimizing Blocking and Nonblocking Reduction Operations for Multicore Systems: Hierarchical Design and Implementation

ORNL Team Members: Manjunath Gorentla Venkata, Pavel Shamis, and Rahul Sampath
Richard L. Graham (Mellanox) and Joshua S. Ladd (Mellanox)

This work proposed a design for implementing blocking and non-blocking reduction collective operations for modern multicore systems. An implementation based on the design performed an order of magnitude better than the state of-the-art on variety of systems including Cray and InfiniBand systems. The Conjugate Gradient solver using this implementation completed over 195% faster, compared to the completion time while using the state-of-the-art. These reduction implementations are integrated into Open MPI, a popular implementation of MPI standard, and we expect to release these implementations publicly as part of future Open MPI release. A paper describing the design, implementation, and evaluation of these reductions has been accepted for publication in IEEE Cluster 2013 conference proceedings.

Read the supporting document [**HERE**].

Tamper-indicating Quantum Seals

ORNL Team Members: Travis Humble, Brian Williams, Toby Flynn, Laura Ann Anderson, Dave Richardson

CSMD, CSED, and MSSED researchers have developed a new technology for the technical verification of non-proliferation treaties. With support from the Defense Threat Reduction Agency (DTRA), the CSMD-led team has deployed quantum information concepts to detect when an intruder tampers with a sealed targets. This is a particular concern for treaty inspectors that need to confirm that the containment and surveillance of a special nuclear material has been uninterrupted. The novelty of the ORNL approach is to use quantum entanglement, a quantum mechanical feature that describes how two spatially disparate systems can exhibit seemingly strong correlations in their behaviors. The ORNL team has now leveraged those effects alongside the no-cloning principle to detect when an intruder is present, thus closing a vulnerability in existing tamper-indication technology.
Unlike classical correlations, which can be both observed and copied, the non-local quantum correlations used by the ORNL team can not be copied and any attempts at doing so destroys the entanglement. By monitoring for the presence of entanglement, the team was able to demonstrate a high probability of detection at a very low false alarm rate. In addition, recent development have laid the ground work for making these quantum verification measurements in real time using customized FPGA-based data collection systems.

Result from this work are featured in a special August issue of IEEE COMSOC Magazine on Quantum Communications. T. S. Humble "Quantum Security for the Physical Layer," IEEE COMSOC Magazine, vol. 51, page 56 (2013)http://ieeexplore.ieee.org/xpl/articleDetails.jsp?arnumber=6576339

Highlights (continued)

Hybrid Programming Using OpenSHMEM and OpenACC

ORNL Team Members: Oscar Hernandez and Matthew Baker
Swaroop Pophale (University of Houston), Jean-Charles Vasnier (CAPS Enterprise), and Haoqiang Jin (NASA)

With high performance systems exploiting multicore and accelerator-based architectures on a distributed shared memory system, heterogenous hybrid programming models are the natural choice to exploit all the hardware made available on these systems. Previous efforts looking into hybrid models have primarily focused on using OpenMP directives (for shared memory programming) with MPI (for inter-node programming on a cluster), using OpenMP to spawn threads on a node and communication libraries like MPI to communicate across nodes. As accelerators get added into the mix, and there is better hardware support for PGAS languages/APIs, this means that new and unexplored heterogenous hybrid models will be needed to effectively leverage the new hardware. In this paper we explore the use of OpenACC directives to program GPUs and the use of OpenSHMEM, a PGAS library for one- sided communication between nodes. We use the NAS-BT Multi-zone benchmark that was converted to use the OpenSHMEM library API for network communication between nodes and OpenACC to exploit accelerators that are present within a node. We evaluate the performance of the benchmark and discuss our experiences during the development of the OpenSHMEM +OpenACC hybrid program.

Software-defined Quantum Communication

ORNL Team Members: Travis Humble, Ron Sadlier, Brian Williams

CSMD researches have developed a new paradigm for leveraging the benefits of quantum communication. While quantum communication protocols like teleportation, entanglement swapping, and QKD are exciting possibilities for today's quantum communication engineers, these protocols are often exotic and unfamiliar to the end user. In addition, protocol implementation is often tightly coupled to the underlying physics, which makes tuning or reconfiguring the communication system difficult and costly.

The CSMD-led team has developed a paradigm for highly reconfigurable quantum communication systems based on software-defined quantum communication. Like its classical namesake, software-defined quantum communication uses software layers to isolate functional concerns and maintain the reusability and extensibility of prior implementation. The team has recently demonstrated their methodology in the design of a super-dense coding communication system, which is a highly efficient quantum protocol for sending messages between users. The work was funded by the Defense Threat Reduction Agency, which uses the software-defined approach to design sensor and communication terminals.
Results from this work are highlighted in a news release from the optical society SPIE and part of an invited presentation at Quantum Communications and Quantum Imaging XI (August, 2013) http://spie.org/x102597.xml

Adiabatic Quantum Programming

ORNL Team Members: Travis Humble, Alex McCaskey, Ryan Bennink, Jay Billings, Ed D'Azevedo, Blair Sullivan, Christine Klymko, Had Seddiqi

With the availability of first generation quantum computers, questions of programming and benchmarking are at the forefront of quantum computer science. A recent CMSD-led effort is helping address these questions by developing an integrated development environment for quantum computing. Funded by the Lockheed Martin Corporation, the ORNL team has developed JADE, or the Jade Adiabatic Development Environment, for managing the complexity of quantum programming. JADE allows users to specify input problems, control instructions, and processor configurations to generate run-time programs. JADE also interfaces with a computational backend that enables simulation of the quantum programs. Such numerical simulations provide detailed diagnostics about program behavior and computational complexity that are needed for building next generation quantum information systems.

Results from this work are available on arxiv preprint server T. S. Humble, A. J. McCaskey, R. S. Bennink, J. J. Billings, E. F. D'Azevedo, B. D. Sullivan, C. F. Klymko, and H. Seddiqi, "An Integrated Development Environment for Adiabatic Quantum Programming," (preprint, 2013), http://arxiv.org/abs/1309.3575

Highlights (continued)

Near Real-time Data Analysis of Core-collapse Supernova Simulations with Bellerophon 1.2

ORNL Team Members: Eric Lingerfelt, Bronson Messer (PI)

Core-collapse supernovae are nature's mechanism for producing the elements heavier than oxygen, which make up our bodies and the world around us. By designing and implementing multi-dimensional, multi-physics codes, like CHIMERA, scientists can leverage the power of supercomputing platforms to explore this phenomenon. CHIMERA's complexity, pace of ongoing development and widely distributed collaborators present many challenges. In order to address those challenges, a multi-tier software system, Bellerophon, has been implemented to meet the verification, data analysis and management needs of CHIMERA's code development team. Since its initial release in April 2010, Bellerophon has enabled the CHIMERA team to discover and isolate multiple bugs and other subtle issues. These capabilities have provided a direct impact on simulation results and facilitated several publications. [more]

CASL Achievements

The Consortium for Advanced Simulation of Light Water Reactors (CASL) was established as the first U.S. Department of Energy (DOE) Innovation Hub, and was created to accelerate the application of advanced modeling and simulation (M&S) to the analysis of nuclear reactors [1]. CASL started operations on July 1, 2010, at its Oak Ridge National Laboratory (ORNL) headquarters in collaboration with ten core partners (ORNL, Idaho National Laboratory (INL), Los Alamos National Laboratory, Sandia National Laboratories, Electric Power Research Institute, Westinghouse Electric Company (WEC), Tennessee Valley Authority (TVA), North Carolina State University, University of Michigan, and Massachusetts Institute of Technology). CASL applies existing M&S capabilities and develops advanced capabilities to create a usable environment for predictive simulation of light water reactors (LWRs). This environment, known as the Virtual Environment for Reactor Applications (VERA), incorporates science-based models, state-of-the-art numerical methods, modern computational science and engineering practices, and uncertainty quantification (UQ) and validation against data from operating pressurized water reactors (PWRs), single-effect experiments, and integral tests.

CSMD staff have been key contributors to CASL since its inception, with Computational Engineering and Energy Science (CEES) Group Leader John Turner serving as Lead of the Virtual Reactor Integration (VRI) Focus Area and staff from the CEES, Computer Science, and Applied Math groups contributing to CASL goals.

Some recent CASL achievements of note include:

- June 30, 2013: Deployment of VERA to Westinghouse Nuclear as CASL's first Test Stand. Ross Bartlett (CEES) was recognized for his efforts to ensure the success of this deployment with a Significant Event Award.
- July 10, 2013: Simulation of reactor startup tests for TVA's Watts Bar Unit 1 using VERA, and comparison with measured operational data [2].
- September 20, 2013: Limited beta release of VERA components through the Radiation Safety Information Computational Center [3].

As CASL begins to transition from development to deployment of technologies, the VRI Focus Area was renamed Physics Integration (PHI), with Jess Gehin (ORNL/NSTD) as Focus Area Lead. Dr. Gehin was formerly Lead for the Advanced Modeling Applications (AMA) Focus Area. Dr. Turner assumed the role of Chief Computational Scientist for CASL.

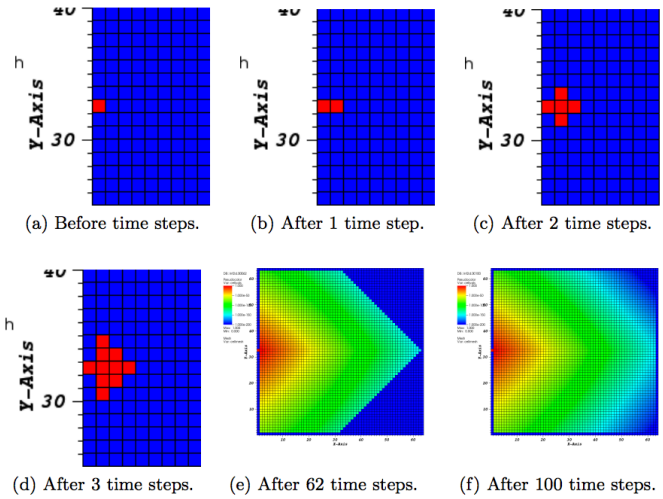
[1] http://www.casl.gov/
[2] http://www.ornl.gov/ornl/news/news-releases/2013/casl-milestone-validates-reactor-model-using-tva-data
[3] https://rsicc.ornl.gov/

Highlights (continued)

Tracking a Value's Influence on Later Computation

ORNL Team Member: Phil Roth

Understanding how a program behaves is important for effective program development, debugging, and optimization, but obtaining the necessary level of understanding is usually a challenging problem. One facet of this problem is to understand how a value (the content of a variable at a particular moment in time) influences other values as the program runs.



(a) Before time steps. (b) After 1 time step. (c) After 2 time steps.

(d) After 3 time steps. (e) After 62 time steps. (f) After 100 time steps.

Value influence propagation for two-dimensional heat transfer application, starting with a single value on the boundary of the problem state array.

To help developers understand value influence for their programs, we are developing a tool that allows a user to tag a value as being of interest, and then track the influence of that value as it, or values that were derived from it, are used in later computation, communication, and I/O. We believe that understanding how a value's influence propagates will enable algorithm designers to more easily identify optimizations such as the removal of unnecessary computation and communication. Our tool supports tracking value influence in multithreaded programs, and we are currently implementing support for applications that use MPI two-sided and collective operations for communication and synchronization.

This work is being done as part of the Institute for Sustained Performance, Energy, and Resilience (SUPER) project of the DOE Office of Science's Scientific Discovery through Advanced Computing program.

Read the supporting document [**HERE**].

Software Releases

INDDGO

Version 2.0 of INDDGO (Integrated Network Decomposition & Dynamic programming for Graph Optimization problems) was released. This release includes major new functionality for the calculation of statistics on graphs. Blair Sullivan of NCSU is primarily responsible for the project. For this release, significant contributions we made by the ESSC Benchmarks team consisting of Matt Baker, Sarah Powers, Jonathan Schrock, and Josh Lothian. More information on INDDGO can be found at: https://github.com/bdsullivan/INDDGO

Gleipnir

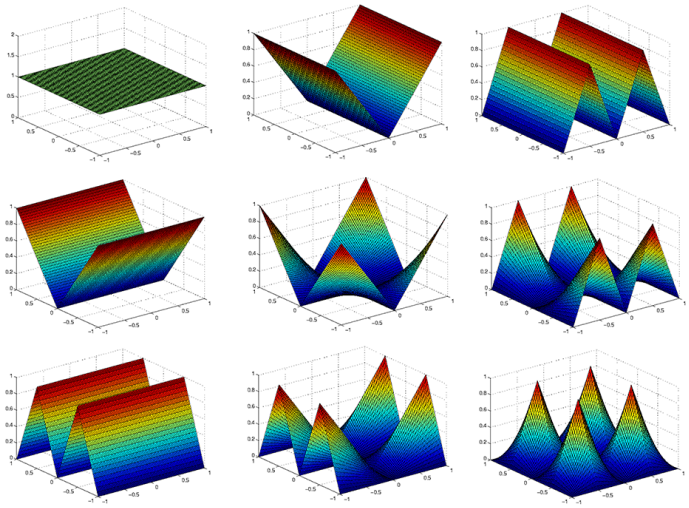
Gleipnir is a memory tracing tool, built as a plug-in for the Valgrind Binary Instrumentation framework. Gleipnir maps memory access information to source code variables/structures (using debug-information or user-defined dynamic regions using client-interface calls). The goal of Gleipnir is to expose application memory access behavior for optimization/analysis purposes. This release provides better support for MPI applications and larger codes. Contact: Tomislav Janjusic, janjusict@ornl.gov [(svn r2568) (http://csrl.unt.edu/gleipnir)]

HERCULES 2.3

HERCULES is an Open64-based, PROLOG-backed, system for program constraint programming and customizable, user-level, transformation formulation. In addition to the core system, it offers a source code base scanner for patterns (hscan) and numerous transformation directives in an F90 compiler (hslf90). Contact: Christos Kartsaklis, kartsaklisc@ornl.gov [svn (r344)]

TASMANIAN

To overcome the challenges of applying Uncertainty Quantification to scientific problems, the Predictive Math Team at ORNL has developed the The Toolkit for Adaptive Stochastic Modeling and Non-Intrusive ApproximatioN (TASMANIAN), which is a feature-rich environment for extreme-scale UQ. TASMANIAN v.1.0 includes the team's adaptive sparse grid stochastic collocation approaches, constructing from both global (hierarchical Lagrange) and local (multi resolution wavelets) basis functions. Moreover, the toolkit also includes a massively scalable implementation of the DiffeRential Evolution Adaptive Metropolis (DREAM) algorithm for accelerating Markov Chain Monte Carlo (MCMC) convergence, used in all parameter estimation and Bayesian inference algorithms. [more]



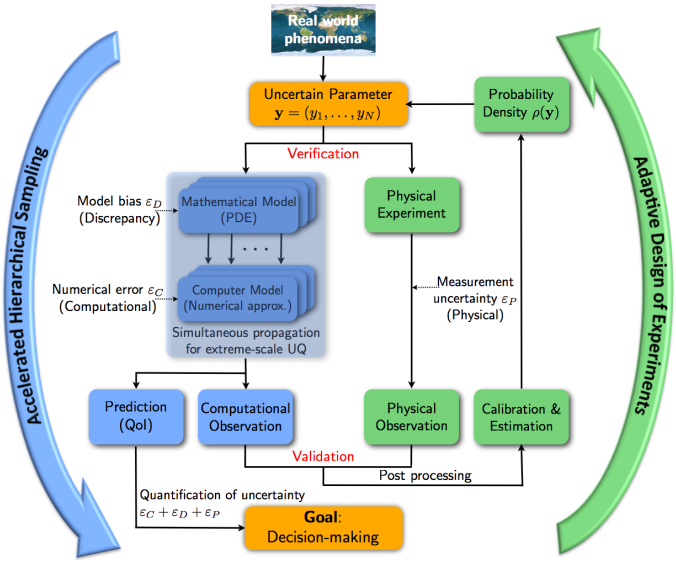
An example of two dimensional hierarchical basis functions used for interpolation. The basis is build from tensor products of one dimensional piece-wise linear functions. The hierarchical properties combined with the local support allow for adaptive interpolation of problems with sharp behavior.

New Funding

A Mathematical Environment for Quantifying Uncertainty: Integrated aNd Optimized at the eXtreme-scale (EQUINOX)

Awarded in response to Lab 13-895: Uncertainty Quantification Methodologies for Enabling Extreme-Scale Science

The ORNL-lead team proposed to establish a modern mathematical and statistical foundation that will enable next-generation, complex, stochastic predictive simulations. Such a foundation is critical to realizing the potential of future computing platforms, including exascale, and will ultimately enable scientists to address a fundamental question, namely "how do the uncertainties ubiquitous in all modeling efforts affect our predictions and understanding of complex phenomena?"



The principal investigator (PI) and coordinator of the combined research efforts of EQUINOX is Clayton Webster (ORNL) with co-PIs Rick Archibald (ORNL), Max Gunzburger (Florida State University), Eric Phipps (Sandia National Labs) and Jeff Wu (Georgia Tech). Additional team members from ORNL include: Cory Hauck, Sreekanth Pannala, Miroslav Stoyanov and Guannan Zhang. Our collaborative approach to uncertainty quantification (UQ) combines novel paradigms in applied mathematics, statistics and computational science into a unified framework, which we call an Environment for Quantifying Uncertainty: Integrated aNd Optimized at the eXtreme-scale (EQUINOX). These includes:

1. Novel adaptive hierarchical approaches for low-discrepancy sampling with sufficient volumetric coverage of the input density; interpolation and approximation in those regions; and detection of events, including rare events, in high-dimensional parameter spaces;
2. Advanced multi-level methods for alleviating the complexity and accelerating the solutions of both deterministic and stochastic extreme-scale solvers;
3. A revolutionary, architecture-aware, UQ paradigm to evaluate samples in parallel through a multi- level embedded propagation scheme whereby collections of samples are executed asynchronously and samples within each collection are propagated simultaneously at the node and processor core levels;
4. Innovative, adaptive and robust experimental design strategies that intelligently gather data from both computer simulations and physical experiments so as to reduce variability in the estimate of the unknown parameters and the uncertainty in predicted responses.

We expect EQUINOX to have substantial impact on scientific discovery, engineering technology and probabilistic risk assessment.

Extreme-scale Algorithms & Solver Resilience (EASIR)

Awarded in response to Lab 12-742: Resilient Extreme-Scale Solvers

As DOE moves towards the Leadership-class machines of the next 5-10 years, algorithms are going to face significant challenges due to: extreme concurrency, complex memory hierarchies, costly data movement, a steep rise in fault rates, and heterogeneous processor architectures. In the face of these challenges, major innovations in algorithm design will be required just to achieve acceptable productivity on future DOE Leadership computers, let alone realize their full promise.

To address this mission critical challenge, a team lead by Al Geist (ORNL) and Mike Heroux (SNL) proposed to create the Extreme-scale Algorithms & Solver Resilience (EASIR) project that focuses on delivering scalable, resilient, and communication and synchronization reducing solver algorithms that will be necessary to achieve performance and resilience on future extreme-scale platforms. Co-investigators on EASIR include Jim Demmel (University of California Berkeley), Jack Dongarra (University of Tennessee), and Bill Gropp (University of Illinois), as well as additional team members from ORNL, including: Bobby Philip, Miroslav Stoyanov, and Clayton Webster.

New Funding (continued)

The EASIR project will advance the state of the art for scalable, resilient, extreme-scale solvers by:

- Developing communication reducing and synchronization reducing algorithm
- Exploring revolutionary methods of algorithm resilience, including the ability to survive silent errors, and algorithms with tunable reproducibility, i.e. bound the perturbation of results
- Developing algorithms that optimize data movement and increased resilience by exploiting variable (higher and lower) precision arithmetic, and deep memory hierarchies
- Create new algorithms for extreme-scale heterogeneous architectures
- Measure all aspects of performance of these new algorithms, including execution time, memory performance, data movement, faults, reproducibility, and energy consumption
- Investigate tunable reproducibility and its potential tradeoffs with extreme scalability and performance

The solver algorithms developed by the EASIR project will be major enablers in exploiting the future generations of DOE Leadership computers to make scientific breakthroughs. The resulting solver algorithms will provide a breakthrough in state-of-the-art algorithm design for the next generation of high-performance computers, providing support for hybrid systems, and significantly exceeding the performance of currently available solutions.

Hobbes: OS and Runtime Support for Application Composition DOE Exascale Operating and Runtime Systems

ORNL team members: David E. Bernholdt (ORNL PI), Hasan Abbasi, Christian Engelmann, Terry Jones, Scott Klasky, A.B. Maccabe, Philip C. Roth, Geoffroy Vallee, and Jeffrey Vetter

The goal of the Hobbes operating system and runtime (OS/R) is to define the core of the system software stack, which can remain fixed as HPC hardware continues to evolve. We will identify and focus on a small set of abstractions that match the resource management challenges of extreme-scale platforms.

We expect future applications to increasingly be composites of today's applications in complex, possibly tightly-coupled workflows. Hobbes participants, led by ORNL, will explore efficient support for application composition at the OS/R level, while minimizing the changes to applications. Virtualization will also play a prominent role in Hobbes, both to provide isolation between application components, and to facilitate portability of the Hobbes environment to non-HPC systems. ORNL also leads the resilience and global information bus areas of the project, and participates in the scheduling and energy/power areas.

The project, which is led by SNL, also includes Georgia Tech, Indiana University, LANL, LBNL, NC State University, Northwestern University, University of Pittsburgh, University of Arizona, UC Berkeley, and University of New Mexico.

Technologies and Tools for Synthesis of Source-to-Sink High-Performance Flows

Principal Investigator: N.S.V. Rao, Lead by Oak Ridge National Laboratory in collaboration with Argonne National Laboratory and University of Memphis

A number of Department of Energy science applications, involving exascale computing systems and large experimental facilities, are expected to generate large volumes of data, in the range of petabytes to exabytes, which will be transported over wide-area networks for the purpose of storage, visualization, and analysis. In support of these applications, the objectives of this project are to (1) develop and test the component technologies and their synthesis methods to achieve source-to-sink high-performance flows, and (2) develop tools that provide these capabilities to users and applications. In terms of the former, we develop (1) optimization methods that align and transition multiple storage flows to multiple network flows on multicore, multibus hosts; and (2) edge and long-haul network path realization and maintenance using advanced provisioning methods including OSCARS and OpenFlow. We also develop synthesis methods that combine these individual technologies to compose high-performance flows using a collection of constituent storage-network flows, and realize them across the storage and local network connections as well as long-haul connections. These solutions will be tested using (1) 100 Gbps connection(s) between Oak Ridge National Laboratory (ORNL) and Argonne National Laboratory (ANL) with storage systems supported by Lustre and GPFS file systems with an asymmetric connection to University of Memphis (UM); and (2) ORNL testbed with multicore and multibus hosts, switches with OpenFlow capabilities, and network emulators.

This project is funded by the Department of Energy, High-Performance Networking Program

New Funding (continued)

Computational Catalytic Pyrolysis Consortium

ORNL team members: Stuart Daw and Sreekanth Pannala

This project, funded by EERE Bioenergy Technologies Office (BETO) at ~$3M/year, will help meet the BETO's 2017 target of $1.56/ gallons of diesel or gasoline by addressing critical technical barriers to the production of refinery-ready pyrolysis oil. The technical barriers from the Multi-Year Program Plan addressed are:

a) Pyrolysis of Biomass and Bio-Oil Stabilization and
b) Fuel Synthesis and Upgrading.

Specifically, this project lead by ORNL (with Stuart Daw as PI and CSMD's Sreekanth Pannala as co-PI) will focus on catalytic fast pyrolysis (in-situ and ex-situ) and hydrotreating of fast pyrolysis oil. Techno-economic analysis of catalytic fast pyrolysis has shown that significant process cost reductions can be gained by improvements in the yields of desirable hydrocarbons (gasoline, diesel and jet range) with concomitant reductions in carbon losses due to coke formation and via process intensification by combining pyrolysis and catalytic upgrading. Techno-economic analysis has also shown that improvements in yields and catalyst lifetime, reduction in reaction severity and efficient use of hydrogen are important cost reduction goals for hydrotreating. These goals will be achieved through a close integration of computational modeling with ongoing experimental OBP-funded studies at NREL, PNNL, INL, and ANL.

Application of High Performance Computing for Simulating Cycle to Cycle Variation in Dual Fuel Engine

ORNL team members: Sreekanth Pannala and Miroslav Stoyanov

GE is working with CSMD researchers Sreekanth Pannala and Miroslav Stoyanov (and other researchers at ORNL) to evaluate ORNL's recently developed sampling methodology to simulate variation in internal combustion engines running on dual fuel (Natural Gas and Diesel) using the high performance computing facilities at ORNL. CFD simulations are planned on 100% diesel and dual fuel combustion. ORNL's methodology is expected to capture the inherent cycle-to-cycle variation in dual fuel combustion. The goal is to establish a computational capability that can predict dilute combustion stability limits using CFD on high performance computing facilities. This capability is to key to design dual fuel locomotive engines for improved operational stability and reliability. CFD results are expected to provide the physical understanding behind the cycle-to-cycle variation in dual fuel combustion. Huge cycle-to-cycle variation can push the engine to knock on one end and misfire or high COV of IMEP on the other end of the stability of combustion. This research is important as this computational methodology can lead to accelerated adoption of natural gas for locomotive propulsion and this is an urgent need driven by the huge natural gas boom in United States. This project also aids national security by reducing dependence on foreign oil. Recently 5M hours have been allotted on Titan for development and early results.

Mechanistic Modeling Framework for Predicting Extreme Battery Response: Coupled Hierarchical Models for Thermal, Mechanical, Electrical and (Electro)chemical Processes

ORNL team members: Srikanth Allu, Sreekanth Pannala, and John Turner

CSMD researchers (Srikanth Allu, Sreekanth Pannala, and John Turner) are part of this collaborative project between Sandia National Labs, Colorado School of Mines, and ORNL. This project is funded by the Energy Storage program within Vehicle Technologies in the DOE EERE office. The objective of this project is to enable computer-aided engineering of batteries, taking advantage of the best available knowledge of material properties, including thermodynamic, transport and kinetic properties of materials as available in the literature or in future experiments. A challenge of many modeling frameworks is inflexibility in response to changing knowledge, and our current Cantera-based framework is built around extensible libraries for thermodynamic, transport and kinetic data that form the basis for electrode and cell-level models. These models will be integrated within the CAEBAT architecture through collaborative development between SNL and ORNL. The team members will expand the functionality of the CAEBAT-I architecture developed at Oak Ridge National Laboratory by incorporating electrochemistry and related physics models. We will be implementing this modeling capability to address two key aspects of Li-

New Funding (continued)

Ion battery chemistry: 1) Modeling the processes that transform chemical energy to thermal energy in abusive scenarios and the associated heat release for both normal operation and abusive conditions and 2) Modeling thermo-electro-mechanical interactions within porous materials that determine the heat, mass and electrical transport processes, addressing cell-level structural evolution under normal operation and abusive conditions.

Isotope Business Office Business Systems Upgrade (IBOBSU) Project

ORNL Team Members: Mitch Ferren, Eric Lingerfelt, Patricia Winter, Donna Ault, Russell Langley, Monty Middlebrook, Justin Rogers, and Michael Smith
Project lead: Mitch Ferren - National Isotope Development Center Isotope Business Office

The National Isotope Development Center (NIDC) is the sole government source of stable and radio-isotope products for science, medicine, security, and applications. The NIDC manages the sale and distribution of these isotopes through the Isotope Business Office (IBO), which is located at ORNL. There are currently three major components to the IBO's business software architecture. The first component is the NIDC website, isotopes.gov, which is a custom-built, database-driven website using PHP and MySQL. The website is highly integrated with the Online Management Toolkit (OMT). The OMT is a web-deliverable, cross-platform Java application providing NIDC staff the capability to quickly and easily modify the Online Catalog of Isotope Products, harvest website statistics, dynamically generate monthly reports, and administer OMT user accounts from any location. The second component is the Isotope Reference Information System (IRIS). IRIS is an archaic, standalone application built with Visual FoxPro that allows NIDC staff to store and access information concerning quotes, orders, inventory, sales, shipments and invoices as well as dynamically generate custom reports. The final component is ORNL's SAP Enterprise Business System. The IBOBSU project's primary goal is the reduction of these three independent systems to two systems via two concurrent tasks. Task 1: Business System Conversion (led by Winter) will streamline the IBO's current workflow by retiring IRIS and integrating its capabilities and database into the existing ORNL SAP system through customization of SAP modules according to process requirements. Task 2: NIDC Website Enhancements (led by Lingerfelt) focuses on the website and OMT, specifically on delivering a secure online quotation and ordering capability of stable isotopes for preferred customers, an online shopping cart feature for quote requests and preferred customers' quotes and orders, and new OMT software tools for the management of quotes, orders, and preferred customer accounts. A new preferred customer portal at isotopes.gov will also be developed allowing preferred customers the ability to securely monitor the status of orders, browse their quote and order history, and manage their profiles.

This work is funded by the DOE's Office of Nuclear Physics under the Isotope Development and Production for Research and Applications (IDPRA) program.

New Faces in CSMD

Megan Cason

Megan Cason is a research staff member of the Future Technologies Group. Megan's research background incorporates parallel architecture and systems design with the problem of mapping irregular algorithms, e.g. graph traversal and irregular mesh computations. She is currently working on tools for application behavior characterization, benchmarks for evaluating scalable heterogeneous systems performance, and evaluation of runtime middleware for exascale applications.

Sergiy Kalnaus

Sergiy Kalnaus recently joined the CEES group as a joint research associate with UTK/ORNL's Joint Institute for Computational Science. Prior to this position, Dr. Kalnaus was a post-doctoral fellow with the battery materials R&D group and CEES group at ORNL. Dr. Kalnaus is an expert on computational mechanics and he is working on various aspects of the energy storage activities within the CEES group including the CAEBAT development.

Tiffany Mintz

Tiffany Mintz is an R&D Associate in the Computer Science Research Group. Tiffany's research has focused on tools that optimize productivity in scientific application development for parallel and heterogeneous computing platforms. She is currently working on projects to develop data motion cost models for power consumption and researching the tradeoffs between power, execution time and resilience.

Sparsh Mittal

Sparsh Mittal is a postdoctoral research associate at Future Technologies Group. Sparsh holds a PhD from Iowa State University. His research focuses on improving energy efficiency of cache and memory systems in modern processors. He is currently working on designing non-volatile memory architectures for CPU-GPU heterogeneous systems.

Sarat Sreepathi

Sarat Sreepathi is a Computer Scientist in the Future Technologies Group. Sarat's prior work includes design and development of a scalable parallel framework and computational intelligence algorithms for solving complex optimization problems. He is presently focused on application characterization and performance analytics for Exascale Co-Design Centers and I/O optimization.

Community Service

- David E. Bernholdt, reviewer for Parallel Computing
- David E. Bernholdt, reviewer for IEEE International Conference on Computational Science and Engineering (CSE)
- David E. Bernholdt, reviewer for Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (ScalA)
- David E. Bernholdt, reviewer for Workshop on Software Engineering for High Performance Computing in Computational Science and Engineering (SE-HPCCSE)
- Christian Engelmann, reviewer, IEEE Transactions on Parallel and Distributed Systems (TPDS)
- Christian Engelmann, reviewer, International Journal of High Performance Computing Applications (IJHPCA)
- Christian Engelmann, technical program committee member, IEEE International Conference on High Performance Computing and Communications (HPCC)
- Christian Engelmann, technical posters program committee member, International Conference for High Performance Computing, Networking, Storage and Analysis (SC) 2013
- Kate Evans served as a panelist for "Effective Strategies for underrepresented groups" at the National Laboratories Professional Development Workshop (CMD-IT NLPDev 2013), June. 13, 2013.
- Kate Evans spoke to educational groups at Harnessed Atom Curriculum Program, Oak Ridge Institute for Research and Education, through the Department of Nuclear Energy, Oak Ridge, TN, July, 2013.
- Kate Evans spoke to educational groups at Oak Ridge Science Camp for Middle School Students, Oak Ridge Institute for Research and Education, Oak Ridge, TN, July, 2013.
- Kate Evans spoke to educational groups at Austin Peay Governor's school visit, Oak Ridge National Laboratory, Oak Ridge, TN, June, 2013.
- Kate Evans gave the plenary talk at the Math of Planet Earth conference in Melbourne, Australia, July 2013
- Manjunath Gorentla Venkata, program committee member, Workshop on Power-aware Algorithms, Systems, and Architectures (PASA)
- Manjunath Gorentla Venkata, program committee member, 19th IEEE International Conference on Networks.
- Manjunath Gorentla Venkata, program committee member, First OpenSHMEM Workshop: Experiences, Implementations and Tools.
- Chung-Hsing Hsu serves as a program committee member for the 11th IEEE/IFIP International Conference on Embedded and Ubiquitous Computing (EUC-13).
- Chung-Hsing Hsu serves as a program committee member for the First OpenSHMEM Workshop: Experiences, Implementations and Tools.
- Tomislav Janjusic, reviewer, Special issue of 'Advances in Computers' on Data Flow versus Control Flow: Creativity, Design, Application, and Education"
- Seyong Lee, program committee member, ICPADS 2013
- Seyong Lee, external review committee member, ACM PPOPP 2014
- Dong Li, external review committee member, ACM PPOPP 2014
- Dong Li, program committee member, IEEE international conference on BigData
- Dong Li, program committee member, IEEE/IFIP international conference on Embedded and ubiquitous computing
- Philip C. Roth, workshop co-organizer, 2013 International Workshop for Data Intensive Scalable Computing Systems (DISCS-2013)
- Philip C. Roth, SC13 Birds of a Feather committee chair
- Pavel Shamis, reviewer, 19th IEEE International Conference on Networks.
- Sarat Sreepathi, Technical reviewer for Journal of Computing in Civil Engineering, Journal of Water and Climate Change and Journal of Environmental Modeling and Software
- Miroslav Stoyanov co-organized a mini-symposium (Recent Advances in Numerical Methods for Partial Differential Equations with Random Inputs) at the 2013 SIAM Annual Meeting, San Diego, CA.
- Geoffroy Vallee, reviewer, IEEE Transactions on Parallel and Distributed Systems
- Jeffrey Vetter, organizing committee member, DOE MODSIM Workshop, 2013
- Jeffrey Vetter, program committee member, ACM PPOPP 2014
- Jeffrey Vetter, program committee member, IEEE HiPC 2013
- Clayton Webster organized a mini-symposium (Recent Advances in Numerical Methods for Partial Differential Equations with Random Inputs) at the 2013 SIAM Annual Meeting, San Diego, CA.
- Patrick Worley, associate editor, Parallel Computing

Community Service (continued)

Society for Industrial and Applied Mathematics Annual Meeting (July 8th - 12th)

The SIAM Annual Meeting is the largest applied math conference held every year. Guannan Zhang and Miroslav Stoyanov organized a mini-symposium on "Recent Advances in Numerical Methods for Partial Differential Equations with Random Inputs," which is a rapidly growing field that is of great importance to science. There were 12 invited speakers from both national labs and academia including ORNL, Argonne National Lab, Florida State University, University of California, University of Pittsburgh, Virginia Tech, University of Minnesota, Auburn University. The mini-symposium was well attended by an even wider variety of researchers. The mini-symposium gave participants an opportunity to discuss their current work as well as future development of the field.

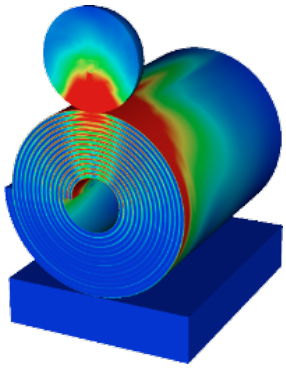
Durmstrang-2 Review

The Fall review for the Durmstrang-2 project was held on September 10-11 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 Durmstrang-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 Fall review. Benchmarks R&D discussion was facilitated by Josh Lothian, Matthew Baker, Jonathan Schrock, and Sarah Powers; Languages and Compilers R&D discussion was facilitated by Matthew Baker, Oscar Hernandez, Pavel Shamis, and Manju Gorentla-Venkata; I/O and FileSystems R&D discussion was facilitated by Brad Settlemyer; Networking R&D discussion was facilitated by Nagi Rao, Susan Hicks, Paul Newman, Neena Imam, and Yehuda Braiman; Power Aware Computing R&D discussion was facilitated by Chung-Hsing Hsu; System Schedulers R&D discussion was facilitated by Greg Koenig and Sarah Powers. A special panel on Lustre was also convened to discuss best practices and path forward. Panelists included both DoD and ORNL members. The topics of discussion during the executive session of the review included continued funding/growth of the program, task progression, and development of performance metrics for the project.

Upcoming events for ESSC include: OpenSHMEM Birds-of-a-Feather session at Supercomputing 2013, OpenSHMEM booth at Supercomputing 2013, and OpenSHMEM Workshop (date to be announced).

CAEBAT Annual Review



The Computer-Aided Engineering for Batteries (CAEBAT) program [1] is funded through the Vehicle Technologies (VT) program office within the DOE Office of Energy Efficiency and Renewable Energy (EERE). This program, led by NREL and including industry and university partners, is developing computational tools for the design and analysis of batteries with improved performance and lower cost. CSDM staff in the Computational Engineering and Energy Science (CEES) and Computer Science (CS) groups are leading development of the shared computational infrastructure used across the program, known as the Open Architecture Software (OAS), as well as defining standards for input and battery "state" representations [2].

On Aug. 27, 2013, the ORNL team (Sreekanth Pannala, Srdjan Simunovic, Wael Elwasif, Sergiy Kalnaus, Jay Jay Billings, Taylor Patterson, and CEES Group Leader John Turner) hosted the CAEBAT Program Manager, Brian Cunningham, at ORNL. This visit served as an annual review for the ORNL CAEBAT effort, and provided a venue for the team to demonstrate progress in simulation capabilities, including an initial demonstration of the use of the NEAMS Integrated Computational Environment (NiCE) with OAS [3].

[1] http://www.nrel.gov/vehiclesandfuels/energystorage/caebat.html
[2] http://energy.ornl.gov/CAEBAT/
[3] http://sourceforge.net/apps/mediawiki/niceproject/index.php?title=CAEBAT

Community Service (continued)

OpenACC Meeting

September 24-26, 2013

The Computer Science Research Group at ORNL hosted the OpenACC Face-to-Face Workshop. OpenACC is a directive-based HPC parallel programming model, designed for performance on - and performance portability across - many types of platforms (e.g., GPUs, many-core and multi-core). OpenACC is complementary to existing HPC programming models including OpenMP, MPI, CUDA and OpenCL. Members of the OpenACC committee develop scientific applications used on accelerator-based supercomputers such as our own Titan. The Workshop was attended by leading experts and researchers in accelerator programming from Cray, PGI, CAPS, ORNL, the technical University of Dresden, the University of Houston, the University of Oregon, the Swiss National Supercomputing Center, NOAA, the Tokyo Institute of Technology, and Allinea.

Participating scientific application developers presented their experiences with OpenACC, and future needs were identified. The last two days of the workshop were spent on planning the implementation of new features in OpenACC, such as transfer of complex data structures to the accelerator, accommodating C++ features, a tools API, and open-source compiler efforts.

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

2013 Christian Engelmann, program chair

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

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

Awards and Recognition

Federal Laboratory Consortium (FLC) 2013 Interagency Partnership Award Recognition

ORNL researchers Jitendra Kumar, Richard Mills, and Forrest Hoffman were congratulated by the Secretary of Energy, Ernest Moniz, for being named recipients of the 2013 Interagency Partnership Award by the Federal Laboratory Consortium (FLC). The award recognizes laboratory employees and private collaborators who accomplished outstanding work in transferring technology developed in the Federal Laboratory to the commercial marketplace.

Chuck Glover Recognized by MDA

Chuck Glover is the technical lead at the Missile Defense Agency (MDA) for the development of innovative methods for missile defense flight test analysis. MDA has recognized his unique contributions, as shown in the attached documents. Specifically, this involves:

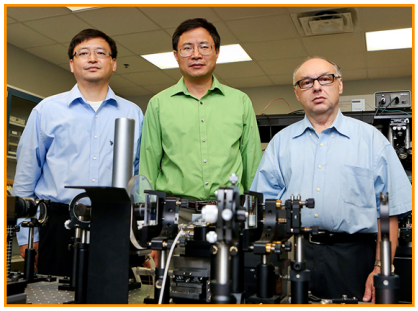
- Austere Challenge-12. This was is a 3 month long Defense Department exercise between the U.S. European Command (EUCOM) and Israeli Warfighters. Chuck was the C2BMC test team lead for this exercise. The results of his contributions will alter how modeling and simulation will be used in this and other DoD exercises, both Nationally and Internationally.
- FAST Eagle-II. This was a 3 months emergency test for the U.S. Central Command (CENTCOM) with U.S. forces in Bahrain, Qatar, Kuwait, and United Arab Emirates. This test included US. THAAD, PATRIOT, Aegis Cruisers and C2BMC. Chuck was the C2BMC test team lead for this test of the U.S missile defense system against Iranian threats. The results from this test provided CENTCOM and International partners with new unmatched capabilities.

Awards and Recognition (continued)

NASA Award

ORNL researchers Jitendra Kumar, Richard Mills, and Forrest Hoffman were presented with the NASA Group Achievement Award for their contributions to the multi-agency ForWarn project.

R&D100 Awards



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

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

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

Jack Dongarra to Receive Ken Kennedy Award for Software Technologies that Power Supercomputers to Tackle Big Scientific Problems

DENVER, CO, October 8, 2013 – Jack Dongarra of the University of Tennessee will receive the ACM-IEEE Computer Society Ken Kennedy Award for his leadership in designing and promoting standards for mathematical software used to solve numerical problems common to high performance computing (HPC). His work has led to the development of major software libraries of algorithms and methods that boost performance and portability in HPC environments, which rely on supercomputers and parallel processing techniques for solving complex computational problems. Dongarra, the Distinguished University Professor at the University of Tennessee, is the founder and director of the Innovative Computing Laboratory at the University, and holds positions at Oak Ridge National Laboratory and the University of Manchester. He will receive the Kennedy Award on November 19 in Denver at SC13, the International Conference on High Performance Computing. [more]

Reuter Wins LDRD Poster Session

The Laboratory Directed R&D program's annual poster session for projects that are to be completed by the end of the fiscal year, September 30, was held in Building 5700's Main Street earlier this week. Principal investigators were on hand Wednesday to discuss their projects.

Of the 74 posters displayed, the LDRD Office selected the best poster in each of three categories: Seed Fund, Director's R&D Fund, and Fellowship (encompassing Weinberg and Wigner). Matthew G. Reuter of the Computer Science and Mathematics Division won the Fellowship category for a project titled "An Accurate and Efficient Computational Methodology for Simulating Disordered Nanoscale Materials."

Awards and Recognition (continued)

Webster Appointed Science Fellow

Clayton Webster was selected as a Kavli Frontiers of Science Fellow in July, 2013, and asked to participate in the German-American Kavli Frontiers of Science symposium, which is jointly organized by the Alexander von Humboldt Foundation and the US National Academy of Sciences (NAS). The symposium brings together the very best young scientists to discuss exciting advances and opportunities in a broad range of disciplines. A committee of NAS members selects the participants from among young researchers who have already made recognized contributions to science, including highly cited papers and recipients of major fellowships and awards. These are highly interdisciplinary symposia emphasizing communication of a wide range of contemporary science topics across the traditional disciplines.

The symposia, which are both national and international in scope, enable emerging and outstanding young scientific leaders to become acquainted with their counterparts in a broad range of disciplines, and to stimulate long-term relationships with their peers. The participants become acquainted with their colleagues in other nations, and in this way build an international network of scientific communication and cooperation. The symposia also serve to inform these young scientists about the challenges and opportunities being addressed at the frontiers of other scientific disciplines, and to broaden their perspectives on the scientific enterprise as a whole.

Researchers Win Gauss Award

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

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

CSMD researcher Bobby Sumpter, along with fellow ORNL researchers Witold Nazarewicz and Stan Wullschleger, has been selected as a 2013 UT-Battelle Corporate Fellow

"Witek, Bobby and Stan are honored both for their individual achievements and for their contributions as mentors and collaborators," Lab Director Thom Mason said. "Their superlative leadership in nuclear physics, computational chemistry and materials, and climate and environmental sciences, respectively, has advanced the frontiers of knowledge across fields of critical importance to ORNL's mission."

Bobby Sumpter leads both the Computational Chemistry & Materials Science group in the Computer Science and Mathematics Division and the Nanomaterials Theory Institute at the Center for Nanophase Materials Sciences. He has been exceptionally productive at the confluence of theory and experiment, working across organizational boundaries to provide theory and modeling leadership across disciplines.

Bobby received his bachelor's degree in chemistry from Southwestern Oklahoma State University and his doctorate in physical chemistry from Oklahoma State University. He has published more than 300 papers with 6,000 citations. [more]

Events

Seminars

- September 30, 2013 - Eric Barton: Fast Forward Storage and Input/Output (I/O)
- September 25, 2013 - James Beyer: OPENMP vs OPENACC
- September 25, 2013 - Michael Wolfe: OPENACC 2.X AND BEYOND
- September 23, 2013 - Jun Jia: Accelerating time integration using spectral deferred correction
- September 19, 2013 - Kenny Gross: Energy Aware Data Center (EADC) Innovations: Save Energy, Boost Performance
- September 17, 2013 - Damien Lebrun-Grandie: Simulation of thermo-mechanical contact between fuel pellets and cladding in UO2 nuclear fuel rods
- September 5, 2013 - Jared Saia: How to Build a Reliable System Out of Unreliable Components
- August 21, 2013 - Hank Childs: Hybrid Parallelism for Visualization and Analysis
- August 13, 2013 - Rodney O. Fox: Quadrature-Based Moment Methods for Kinetics-Based Flow Models
- August 12, 2013 - Lucy Nowell: ASCR: Funding/ Data/ Computer Science
- August 8, 2013 - Carlos Maltzahn: Programmable Storage Systems
- August 7, 2013 - Tiffany M. Mintz: Toward Abstracting the Communication Intent in Applications to Improve Portability and Productivity
- August 2, 2013 - Alberto Salvadori: Multi-scale and multi-physics modeling of Li-ion batteries: a computational homogenization approach
- August 2, 2013 - Michela Taufer: The effectiveness of application-aware self-management for scientific discovery in volunteer computing systems
- July 24, 2013 - Catalin Trenchea: Improving time-stepping numerics for weakly dissipative systems

Upcoming Events

OpenSHMEM Workshop

March 4-6, 2014 Annapolis, Maryland

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

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

Publications/Presentations

Abstract - conference

- Allu, Srikanth (ORNL), Pannala, Sreekanth (ORNL), Kalnaus, Sergiy (ORNL), Elwasif, Wael R. (ORNL), Turner, John A. (ORNL) "Coupled Multi-Physics Model for Li-ion Battery Cells during Impact" EUROMAT 2013 , European Congress and Exhibition on Advanced Materials and Processes, Seville, Spain 9/2013
- Archibald, Richard K. (ORNL) "Characterization of Discontinuities in High-Dimensional Spaces for Arbitrary Data " SIAM Annual 2013, San Diego, California, USA 7/2013
- Li, Dong, Lee, Seyong, Vetter, Jeffrey, "Evaluating the Viability of Application-Driven Cooperative CPU/GPU Fault Detection". In Workshop on Resiliency in High Performance Computing . In conjunction with Euro-Par, 2013
- Radhakrishnan, Balasubramaniam (ORNL), Gorti, Sarma B. (ORNL), Simunovic, Srdjan (ORNL), Clarno, Kevin T. (ORNL) "Co-evolution of microstructure and mechanical properties in structural alloys- Case Studies" 12th US National Congress on Computational Mechanics (USNCCM12), Raleigh, North Carolina, USA 7/2013
- 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, USA 7/2013
- Rao, Nageswara S. (ORNL) "Chaotic maps for robustness estimation of Exascale computations" DOE Applied Mathematics, Albuquerque, New Mexico, USA 8/2013

Abstract - no conference

- D'Azevedo, Ed F. (ORNL), Ku, Seung-Hoe (Princeton Plasma Physics Laboratory (PPPL)), Lang, Jianying (Princeton Plasma Physics Laboratory (PPPL)), Worley, Patrick H. (ORNL) "Algorithm Improvement for Performance" 8/2013
- Humble, Travis S. (ORNL) "Software-defined Quantum Communication" 7/2013

Book

- Mittal, Sparsh (ORNL) "Cache Energy Optimization Techniques For Modern Processors " Scholars' Press, Saarbruecken, Germany ISBN: 978-3-639-51736-1 8/2013

Journal Article

- Ahn, Suk-kyun, Pickel, Deanna L., Kochemba, W. Michael, Chen, Jihua, Uhrig, David, Hinestrosa, Juan Pablo, Carrillo, Jan-Michael, Shao, Ming, Do, Changwoo, Messman, Jamie M., Brown, W. Michael, Sumpter, Bobby G., Kilbey II, S. Michael, “Poly(3-hexylthiophene) Molecular Bottlebrushes via ROMP: Macromolecular Architecture Enhanced Aggregation,” Macro. Lett. 2, 761-765 (2013) DOI: 10.1021/mz4003563.
- Alonzo, José, Kochemba, W. Michael, Pickel, Deanna L., Ramanathan, Muruganathan, Sumpter, Bobby G., Heller, William T., Kilbey II, S. Michael, “Assembly and Organization of Poly(3-hexylthiophene) (P3HT) Brushes and Their Potential Use as Novel Anode Buffer Layers,” Nanoscale 5, 9357-9364 (2013). DOI: 10.1039/c3nr02226a
- Carrillo, J. Michael, Kumar, Rajeev, Goswami, Monojoy, Sumpter, Bobby G., Brown, M., “New Insights into Dynamics and Morphology of P3HT:PCBM Active Layers in Bulk

Heterojunctions," Phys. Chem. Chem. Phys. DOI: 15, 17873-17882 (2013) 10.1039/c3cp53271b.

- Chen, Jihua, Alonzo, Jose, Yu, Xiang, Hong, Kunlun, Messman, Jamie M., Ivanov, Ilia,.Lavrik, Nickolay V., Banerjee, Moloy, Rathore, Rajendra, Sun, Zhenzhong, Li, Dawen, Mays, Jimmy W., Sumpter, Bobby G., Kilbey II, S. Michael, "Grafting-Density Effects, Optoelectrical Properties and Nano-Patterning of Poly(para-Phenylene) Brushes," J. Mater. Chem. DOI: 10.1039/C3TA12745A (2013).
- Gunzburger, Max D. (ORNL), Webster, Clayton G. (ORNL), Zhang, Guannan (ORNL) "An adaptive sparse-grid-based iterative ensemble Kalman filter approach for parameter field estimation" International Journal of Computer Mathematics, 9/2013
- Gunzburger, Max D. (ORNL), Webster, Clayton G. (ORNL), Zhang, Guannan (ORNL) "An Adaptive Wavelet Stochastic Collocation Method for Irregular Solutions of PDEs with Random Input Data" Springer Lecture Notes on CS&E, 9/2013
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- Roth, Philip C. (ORNL) "Tracking a Value's Influence on Later Computation" 6th Workshop on Productivity and Performance, Aachen, , Germany 8/2013
- Tuarob, Suppawong (ORNL), Pouchard, Line Catherine (ORNL), Giles, Lee (Penn state university) "Automatic Annotation of metadata using probabilistic topic modeling" Joint Conference on Digital Libraries, Indianapolis, Indiana, USA 7/2013

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- Wang, Bin (Auburn University, Auburn, Alabama), Wu, Bo (College of William and Mary, Williamsburg, VA), Li, Dong (ORNL), Shen, Xipeng (College of William and Mary, Williamsburg, VA), Yu, Weikuan (ORNL), Jiao, Yizheng (Auburn University, Auburn, Alabama), Vetter, Jeffrey S. (ORNL) "Exploring Hybrid Memory for GPU Energy Efficiency through Software-Hardware Co-Design" International Conference on Parallel Architectures and Compilation Techniques, Edinburgh, United Kingdom 9/2013

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- Evans, Katherine J. (ORNL) "Recent Strategies and Challenges for Simulation and Reproducibility in Climate Modeling" Mathematics of the Planet Earth, Melbourne, Australia
- Li, Dong, "Quantitative Modeling of Data Structure Vulnerability With an Application-Centric Approach," an invited presentation at DOE workshop on Modeling & Simulation of Exascale Systems & Applications, Seattle, WA, September 18, 2013
- Philip, Bobby (ORNL) "AMP: An Object-Oriented Multiphysics Framework" GARUDA-NKN National Partners Meet, Bangalore, India
- Philip, Bobby (ORNL) "An Introduction to Multigrid Techniques: Part 2" CIMPA-UNESCO-MESR-MINECO-NPDE-NBHM Research School on Current Trends in Computational Methods for PDEs, Bangalore, India
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- Roth, Philip C. (ORNL) "Tracking a Value's Influence on Later Computation" 6th Workshop on Productivity and Performance, Aachen, Germany
- Stoyanov, Miroslav K. (ORNL), Webster, Clayton G. (ORNL) " Algorithm Based Software Resilience for Next Generation Extreme Scale Solvers" 2013 DOE Applied Mathematics Program meeting, Albuquerque, New Mexico, USA

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- Boffi, Nicholas M. (ORNL), Hill, Judith C. (ORNL), Reuter, Matthew G. (ORNL) "Estimating the Numerical Bandwidth of the Inverse of a Block Tridiagonal, Block Toeplitz Matrix"
- Brim, Michael J. (ORNL) "Overview of Performance Tools on Titan"
- Chame, Jacqueline (University of Southern California), Hall, Mary W. (University of Utah), Hollingsworth, Jeffrey K. (University of Maryland), Huck, Kevin (University of Oregon), Malony, Allen D. (University of Oregon), Moore, Shirley V. (University of Texas at El Paso), Norris, Boyana (Argonne National Laboratory (ANL)), Oliker, Leonid (Lawrence Berkeley National Laboratory (LBNL)), Roth, Philip C. (ORNL), Williams, Samuel (Lawrence Berkeley National Laboratory (LBNL)), Worley, Patrick H. (ORNL) "SUPER Computer Performance: Analysis and Optimization"
- Chang, Choong-Seock (Princeton Plasma Physics Laboratory (PPPL)), Ku, Seung-Hoe (Princeton Plasma Physics Laboratory (PPPL)), Sugiyama, Linda E. (Massachusetts Institute of Technology (MIT)), Parker, Scott E. (University of Colorado, Boulder), Greenwald, Martin J. (Massachusetts Institute of Technology (MIT)), Tynan, George R. (University of California, San Diego), Kritz, Arnold (Lehigh University, Bethlehem, PA), Stotler, D. (Princeton Plasma Physics Laboratory (PPPL)), Worley, Patrick H. (ORNL) "Extreme Scale Computing of Fusion Phyiscs in the Center for Edge Physics Simulation"
- Evans, Katherine J. (ORNL) "Strategies for using high- resolution global climate models to characterize weather patterns"
- Gu, Lianhong (ORNL), Norby, Richard J. (ORNL), Yang, Xiaojuan (ORNL), Jensen, Anna M. (ORNL), Walker, Anthony P. (ORNL), Warren, Jeffrey (ORNL), Weston, David (ORNL), Hoffman, Forrest M. (ORNL) "Model-Inspired Science Priorities for Evaluating Tropical Ecosystem Response to Climate Change -- Part I: Observations, theoretical process analyses and national and international collaborations"
- Hoffman, Forrest M. (ORNL), Bochev, Pavel B. (Sandia National Laboratories (SNL)), Cameron-Smith, Philip J. (Lawrence Livermore National Laboratory (LLNL)), Easter Jr., Richard C. (Pacific Northwest National Laboratory (PNNL)), Elliott, Scott M. (Los Alamos National Laboratory (LANL)), Grindeanu, Iulian (Argonne National Laboratory (ANL)), Guba, Oksana (Sandia National Laboratories (SNL)), Liu, Xiaohong (Pacific Northwest National Laboratory (PNNL)), Lowrie, Robert B. (Los Alamos National Laboratory (LANL)), Lucas, Donald D. (Lawrence Livermore National Laboratory (LLNL)), Mills, Richard T. (ORNL), Sacks, William J. (National Center for Atmospheric Research (NCAR)), Tautges, Timothy J. (Argonne National Laboratory

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- Kora, Guruprasad H. (ORNL) "KBase Central Data Store and All Biological Data Repository"
- Li, Dong, "Toward Exascale Resilience with A Data-Centric Approach," an invited talk at the department of electrical engineering and computer science, University of Tennessee at Knoxville, TN, September 25, 2013
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- Yang, Xiaojuan (ORNL), Norby, Richard J. (ORNL), Gu, Lianhong (ORNL), Hoffman, Forrest M. (ORNL), Jensen, Anna M. (ORNL), Kumar, Jitendra (ORNL), Maddalena, Damian M. (ORNL), Sun, Ying (University of Texas at Austin), Walker, Anthony P. (ORNL), Warren, Jeffrey (ORNL), Weston, David (ORNL) "Model-Inspired Science Priorities for Evaluating Tropical Ecosystem Response to Climate Change -- Part II: Model simulations and the implications for field experiments"

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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.

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- Computational Chemical and Materials Sciences - Bobby Sumpter
- Computational Earth Sciences - Kate Evans (Interim)
- Computational Engineering and Energy Sciences - John Turner
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LINKS

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Computing and Computational Sciences Directorate - computing.ornl.gov
Oak Ridge National Laboratory - www.ornl.gov

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