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CSMD

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this issue

Highlights P.1
Ongoing Work P.7
LDRD Projects P.8
New Faces P.12
Moving On P.12
Awards P.13
Events P.15
Publications/Presentations P.16
About CSMD P.25

Upcoming Events

SIAM SEAS 2013

The 37th annual meeting of the SIAM Southeastern Atlantic Section will be hosted jointly by the Oak Ridge National Laboratory and the University of Tennessee-Knoxville. The meeting will take place March 22-24, 2013, and will contain the usual combination of plenary talks, minisymposia sessions, and contributed talks and posters.

SOS17 Conference

The SOS 17 Conference will be held on March 25-28, 2013, at the Jekyll Island Club Hotel, Jekyll Island, Georgia.

This year's Conference will explore the intersection between high performance computing and big data. What is it? What are the gaps? What is the state of software for turning data into knowledge?

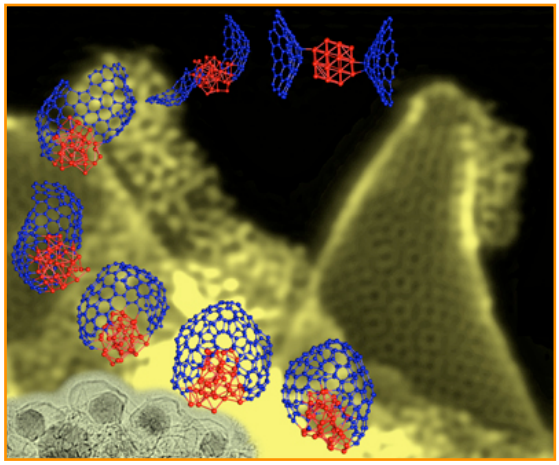
Highlights

High-Temperature Transformation of Fe-Decorated Single-Wall Carbon Nanohorns to Nanooysters: A Combined Experimental and Theoretical Study

The high-temperature conversion of single-wall carbon nanohorns and surface-decorated iron nanoparticles into a new type of nanooyster structure is examined both experimentally and theoretically.

Nanooysters are so-named because iron nanoparticles become enclosed within a single-wall or multiwall carbon capsules resembling pearls at one end of an oyster shell. Quantum chemical molecular dynamics (QM/MD) simulations suggest one possible mechanism by which iron nanoparticles in contact with carbon nanohorn fragments can grow into self-enclosed single-wall nanooysters (SWNOs) by assisting the assembly of dangling carbon bonds accompanied by migration of the metal particle inside the carbon structure. Both the experimental and theoretical results confirm the occurrence of a new hybrid material, a nanooyster, from the nanocones interacting with the iron nanoparticles at elevated temperatures.

New hybrid "nanooysters" consisting of encapsulated metal nanoparticles inside hollow carbon shells, were synthesized by transforming single-wall carbon nanohorns with reactive metals. The nanostructures are



The process by which curved nanocones of carbon (blue) encapsulate Fe nanoparticles (red) to form a new hybrid "nanooyster" material (inset) is shown through snapshots of QM/MD simulations. Background is an aberration-corrected, atomic resolution, Z-STEM image of single wall carbon nanohorns and unconverted graphene flakes which served as the feedstock in the process.

readily produced by rapid, high-temperature annealing in an all-solid-state synthesis approach, pointing the way to the creation of new forms of encapsulated metallic quantum dots with new functional properties in protected, environmentally compatible shells. Understanding how metal nanoparticles can convert curved carbon into new nanostructures such as nanooysters required a novel "nano-enabled materials design" approach, wherein theory, synthesis, and

OAK RIDGE National Laboratory

characterization are used to unravel the atomistic mechanisms driving the formation of this new type of carbon-metal system. This process was recently published in *Nanoscale*. Hollow single-wall carbon nanohorns were first synthesized in a laser vaporization process from pure carbon, then were decorated with metal and rapidly heat-treated with lasers to form the carbon nanooysters. State-of-the-art electron microscopy provided unprecedented characterization of the nanomaterials. Density functional theory-based calculations showed the mechanism by which metal nanoparticles can assist edge coalescence in the nanooyster shell to form a hollow structure.

"High-Temperature Transformation of Fe-Decorated Single-Wall Carbon Nanohorns to Nanooysters: A Combined Experimental and Theoretical Study", K. R. S. Chandrakumar, Jason D. Readle, Chris Rouleau, Alex Puretzky, David B. Geohegan, Karren Morec, Veena Krishnan, Mengkun Tian, Gerd Duscher, Bobby Sumpter, Stephan Irle, Keiji Morokuma, *Nanoscale*. DOI: 10.1039/c0xx00000x.

Acknowledgement of Support:
This research was conducted in part at the Center for Nanophase Materials Sciences (CNMS), and at Oak Ridge National Laboratory's Shared Research Equipment (ShaRE) User Facility, both of which are sponsored by the Scientific User Facilities Division, DOE-BES. Experimental synthesis research supported by the U.S. Department of Energy (DOE), Basic Energy Sciences (BES), Materials Sciences and Engineering Division. The theoretical work was in part supported by a CREST (Core Research for Evolutional Science and Technology) grant in the Area of High Performance Computing for Multiscale and Multiphysics Phenomena from the Japanese Science and Technology Agency (JST). SI acknowledges support by the Program for Improvement of Research Environment for Young Researchers from MEXT of Japan. The computations were performed using the resources of the CNMS and the National Center for Computational Sciences at Oak Ridge National Laboratory.

An Integrated Website and Software System for the National Isotope Development Center

A new database-driven website, isotopes.gov, has been designed and developed for the National Isotope Development Center (NIDC), which is the sole government source of stable and radio-isotope products for science, medicine, security, and applications. Since going live in May 2011, isotopes.gov has provided customers detailed information concerning NIDC activities, funding opportunities, jobs and training, meetings and workshops, outreach and education, production research, and the Isotope Business Office (IBO). The website also hosts the Online Isotope Product Catalog, which allows customers to interactively explore the catalog and submit requests for quotations and new products. In addition to the website, a suite of intra-office software tools, the NIDC Online Management Toolkit (OMT), has been released. The OMT provides NIDC staff the capability to quickly and easily modify the product catalog, harvest website statistics, dynamically generate monthly reports, and administer OMT user accounts.

Developed by Eric Lingerfelt (CSMD) and Michael Smith (Physics), the website has successfully brought the NIDC's web presence for the forefront and encouraged interaction with new and existing customers. It has also served to educate the public on the important role that isotopes play in society. During FY12, for example, the Online Isotope Product Catalog registered 45,000 unique isotope product hits and generated 710 quotation requests. isotopes.gov was also used in Fall 2012 to announce and respond to queries on the auction of 4,000 liters of purified He-3 gas worth $10 million. The OMT facilitates the NIDC's objectives by providing a web-deliverable, cross-platform content management system for the Online Isotope Product Catalog and easy-to-use tools to dynamically generate monthly reports that are used by DOE to guide future isotope production decisions.

This work is funded by the Isotope Development and Production for Research and Applications (IDPRA) subprogram of the Office of Nuclear Physics in the U.S. Department of Energy Office of Science.

Signatures of Cooperative Effects and Transport Mechanisms in Conductance Histograms

ORNL researchers have developed a tractable model for simulating conductance histograms, which are a common form of reporting experimental data on electron transport processes in nanometer-scale systems (e.g., conductance through molecular wires).

M.G. Reuter, M.C. Hersam, T. Seideman, M.A. Ratner

Achievement

We develop a tractable model for simulating conductance histograms, which are a common form of reporting experimental data on electron transport processes in nanometer-scale systems (e.g., conductance through molecular wires). With this model, we can investigate the roles of the various physical parameters on data reported in a conductance histogram. For transport through a single wire, the histogram peak elucidates the mechanism of electron transport. The peak additionally reveals the relative frequencies of these mechanisms if more than one contributes to conduction. A histogram peak from multiple wires indicates the presence of cooperative effects (crosstalk)

between the wires and also encodes information on the underlying conduction channels. Before this study, this information, albeit present in existing experimental data, was ignored.

Significance

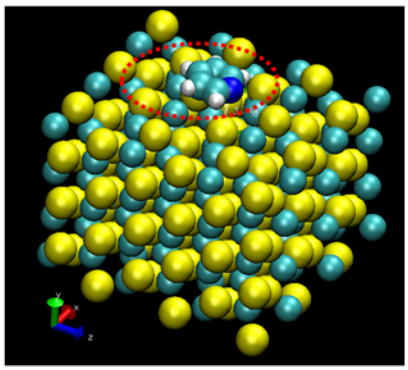
This work helps build a bridge between theory/computation and experiment to better understand electron transport processes through nanometer-scale systems. Theory has generally focused on conductance through a molecule in a fixed configuration, whereas, in most cases, experiment cannot determine, let alone control, the molecular configuration. Our general model adds, for the first time, elements of stochasticity, which connects well-established theory with observable experimental data. We find that, in addition to an average molecular conductance, conductance histograms reveal transport mechanisms and cooperative effects. Finally, this work paves the way to infer theoretical parameters from experimental data.

Credit - This work was published in *Nano Lett*. This research was supported in part (i) by the Department of Energy Computational Science Graduate Fellowship Program, (ii) by the Eugene P. Wigner Fellowship Program, and (iii) at the Center for Nanophase Materials Sciences, which is sponsored at the Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

"Signatures of Cooperative Effects and Transport Mechanisms in Conductance Histograms", M.G. Reuter, M.C. Hersam, T. Seideman, M.A. Ratner, Nano Lett. (2012), DOI: 10.1021/nl204379j.

In Situ Formation of Pyridyl-Functionalized Poly(3-hexylthiophene)s via Quenching of the Grignard Metathesis Polymerization: Toward Ligands for Semiconductor Quantum Dots

CSMD researcher Bobby Sumpter was part of a team that demonstrated a facile one-pot method for preparing 2-pyridyl and 3-pyridyl P3HTs with high abundance of monofunctional products is established via an examination of the kinetics of the end-functionalization quenching reaction with lithium chloride complexes of 2- and 3-pyridyl Grignard reagents. Density functional theory calculations guide the selection of pyridine as the end group, which provides the capacity to ligate cadmium selenide (CdSe) nanocrystals and arrests aggregation upon thermal annealing when dispersed in a P3HT matrix. The ability to manipulate end group compositions coupled with the propensity of pyridyl-functionalized P3HTs to ligate semiconductor quantum dots (SQDs) opens new possibilities for tuning the morphology of conjugated polymer/SQD blends.



Binding energies calculated using density functional theory (DFT) were used to guide selection of pyridyl end groups for synthetic development.

"In Situ Formation of Pyridyl-Functionalized Poly(3-hexylthiophene)s via Quenching of the Grignard Metathesis Polymerization: Toward Ligands for Semiconductor Quantum Dots" W. Michael Kochemba, Deanna L. Pickel, Bobby G. Sumpter, Jihua Chen, S. Michael Kilbey
Chem. Mater. DOI: 10.1021/cm302915hr.

International Community Charts Course for Land Model Benchmarking

ORNL Team Member: Forrest Hoffman

Following on the heels of early efforts to develop systematic evaluation approaches for the land component of climate models, including the DOE-sponsored Carbon-Land Model Intercomparison Project (C-LAMP), an international group of researchers assembled to define a common framework for benchmarking land model performance. Participants identified challenges to routine model performance characterization and proposed a benchmarking framework designed to measure model prediction skills for simulating ecosystem responses and feedbacks to climate change based on comparison with best-available observations. In a recent paper, candidate benchmarks for simulation of biophysical processes, biogeochemical cycles, and vegetation dynamics were proposed as the baseline standards for the International Land Model Benchmarking (ILAMB) Project. Adoption of this benchmarking framework will standardize model assessments, encourage routine evaluation of model performance throughout development, and provide a basis for quantifying model improvements.

Reference: Luo, Y. Q., J. T. Randerson, G. Abramowitz, C. Bacour, E. Blyth, N. Carvalhais, P. Ciais, D. Dalmonech, J. B. Fisher, R. Fisher, P. Friedlingstein, K. Hibbard, F. Hoffman, D. Huntzinger, C. D. Jones, C. Koven, D. Lawrence, D. J. Li, M. Mahecha, S. L. Niu, R. Norby, S. L. Piao, X. Qi, P. Peylin, I. C. Prentice, W. Riley, M. Reichstein, C. Schwalm, Y. P. Wang, J. Y. Xia, S. Zaehle, and X. H. Zhou (2012) "A Framework for Benchmarking Land Models." Biogeosci., 9(10):3857–3874. doi:10.5194/bg-9-3857-2012.

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Highlights (continued)

Keeneland Project Deploys GPU Super for NSF

HPCWire

ATLANTA, Nov. 14 – Georgia Tech, along with partner research organizations on the Keeneland Project, including the University of Tennessee-Knoxville, the National Institute for Computational Sciences and Oak Ridge National Laboratory, announced today that the project has completed installation and acceptance of the Keeneland Full Scale System (KFS). This supercomputing system, which is available to the National Science Foundation (NSF) scientific community, is designed to meet the compute-intensive needs of a wide range of applications through the use of NVIDIA GPU technology. In achieving this milestone, KFS is the most powerful GPU supercomputer available for research through NSF's Extreme Science and Engineering Discovery Environment (XSEDE) program.

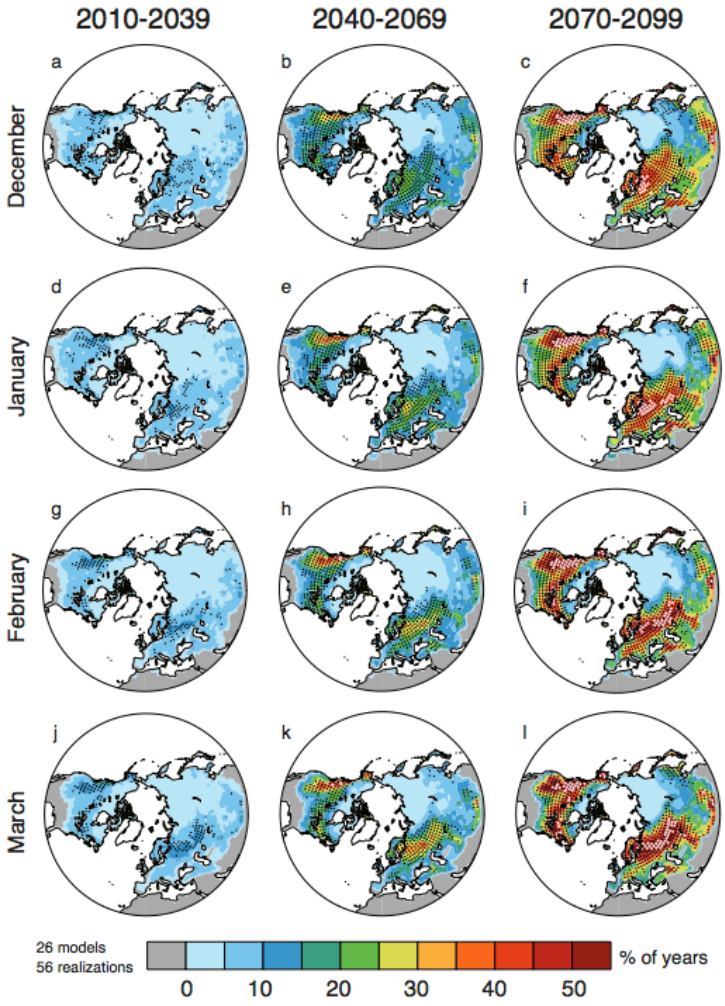
"Keeneland provides an important capability for the NSF computational science community," says Jeffrey Vetter, Principal Investigator and Project Director, with a joint appointment to Georgia Tech's College of Computing and Oak Ridge National Laboratory. "Many users are running production science applications on GPUs with performance that would not be possible on other systems."

Scientists will be able to use the resource to create breakthroughs in many fields of science. For the past 20 months, the Keeneland Initial Delivery System (KIDS) has been used for research in both computer science and computational science, and has included applications in astronomical sciences, atmospheric sciences, behavioral and neural sciences, biological and critical systems, materials research and mechanical and structural systems, along with many other application areas. Much of the research will continue on KFS. Click HERE to read more.

CSMD Researcher Moetasim Ashfaq published in Nature Climate

CSMD researcher Moetasim Ashfaq's paper "Response of snow-dependent hydrologic extremes to continued global warming" has been published by Nature magazine's online presence Nature Climate Change.

The paper focuses on the impact of global warming on snow accumulation and the subsequent influence on water availability (for natural and human systems) in the Northern Hemisphere. Click HERE to read the full article.



Percentage of years with December, January, February and March SWE below the simulated 1976-2005 minimum in the three periods of the RCP 8.5 simulations (56 realizations from 26 models; Table S1).
Following IPCC (2007), stippling indicates areas where the magnitude of the multi-model ensemble mean occurrence divided by the multi-model standard deviation of occurrence exceeds 1.0 (black symbols) or 2.0 (white symbols). Grey denotes areas where at least half of the realizations have a minimum March SWE of zero in the 1976-2005 period.

Highlights (continued)

Advanced Research Projects Agency-Energy Funding

Hsin Wang (MSTD), Srikanth Allu and Sreekanth Pannala

DOE is distributing $43 million in funding from the department's Advanced Research Projects Agency-Energy to 19 new ARPA-E projects, <http://home.ornl.gov/general/ORNL_Today/%28http:/energy.gov/articles/arpa-e-announces-43-million-transformational-energy-storage-projects-advance-electric%29> and a pair of ORNL researchers have $1 million for their project titled Temperature Regulation of Lithium-Ion Cells.

ORNL's Hsin Wang and Sreekanth Pannala are collaborating with Farasis Energy Inc. to develop an innovative battery design to more effectively regulate destructive hot-spots that develop during use. The improvement in transporting heat away from active materials in the battery is expected to increase the battery's life and reduce the system cost associated with thermal management.

"This latest round of ARPA-E projects seek to address the remaining challenges in energy storage technologies, which could revolutionize the way Americans store and use energy in electric vehicles, the grid and beyond, while also improving access to energy for the U.S. military at forward operating bases in remote areas," says Secretary of Energy Steven Chu. "These cutting-edge projects could transform our energy infrastructure, dramatically reduce our reliance on imported oil and increase American energy security."

SUNSHOT BRIDGE Project

In a push to lower the cost of solar power, DOE has funded two projects at Oak Ridge National Laboratory focused on improving solar receiver performance.

One of the projects went to CSMD researcher Sreekanth Pannala for $450,000 with the University of Colorado as the lead and the National Renewable Energy Laboratory as a partner, to fund research on computational optimization of solar receiver designs. Using tools available through ORNL's Oak Ridge Leadership Computing Facility, the project will employ ORNL's expertise in high performance computing and computational granular flows to study high-temperature, inexpensive granular materials for concentrating solar power technologies.

Battery Simulation Tool Released

Srikanth Allu, Wael Elwasif, Srdjan Simunovic, Sreekanth Pannala and John Turner

Given the complex requirements for developing electrical energy storage devices for future transportation needs, a predictive simulation capability is needed that can guide rapid battery design by considering performance and safety implications of different chemistry and materials choices. With such models not currently in existence, the goal of the Vehicle Technology Program's Computer Aided Engineering for Batteries (CAEBAT) program is to do just that – create simulation tools for designing batteries. The program is led by the National Renewable Energy Laboratory with ORNL and several industrial partners.

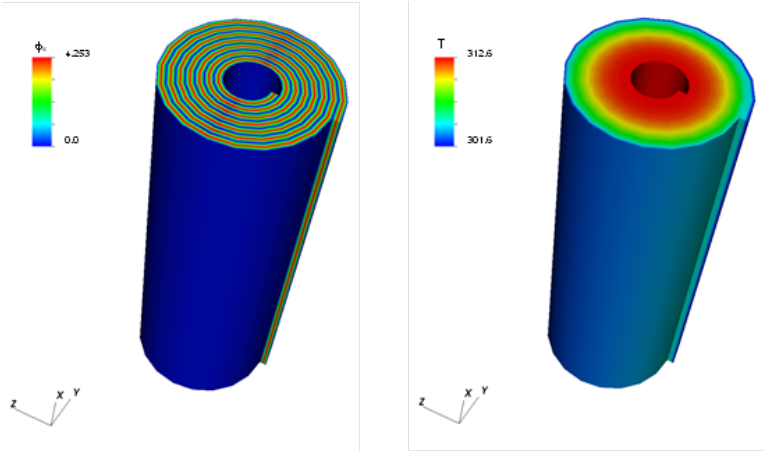


Figure 1: Sample results for current-collector resolved cylindrical cell (electrical potential on the left and the temperature on the right).

Through its role with the CAEBAT project, ORNL is developing a flexible, robust, and computationally scalable open-architecture framework that enables seamless multi-scale and multi-physics simulations of battery performance and safety. The project has four main components: a) open architecture software (OAS), the base computational infrastructure; b) virtual integrated battery environment (VIBE), the OAS framework along with physics and support components and the adapters; c) BatteryML, the standard for specifying input; and d) battery state, the state file(s) to transfer information between the components.

In late October, the ORNL team released a Beta version of CAEBAT OAS framework to industry partners. This version has all the capabilities to do electrochemical-electrical-thermal simulations of a pouch or a cylindrical cell. Watch for progress updates as the teams works closely with partners in the days ahead.

A New Era in Automotive Engine Development Driven by HPC

Wael Elwasif, Srdjan Simunovic, Miro Stoyanov, Clayton Webster and Sreekanth Pannala from CSMD; Robert Wagner, Dean Edwards, Charles Finney and Stuart Daw from ETSD

CSMD researcher Sreekanth Pannala was interviewed about high performance computing's role in the development of new engines.

Highlights (continued)

Says Pannala, “Hundreds of LES simulations of in-cylinder combustion running in parallel using innovative sampling algorithms on massively parallel computers such as Jaguar, provides the researchers with unprecedented data related to cycle-to-cycle variations, allowing us to better comprehend the factors that cause these variations. This open research will provide Ford with knowledge the company can use to create enhanced engine systems designs that enable robust combustion at high EGR rates. The bottom line – greater fuel efficiency and reduced emissions.”
Click HERE to read the full article

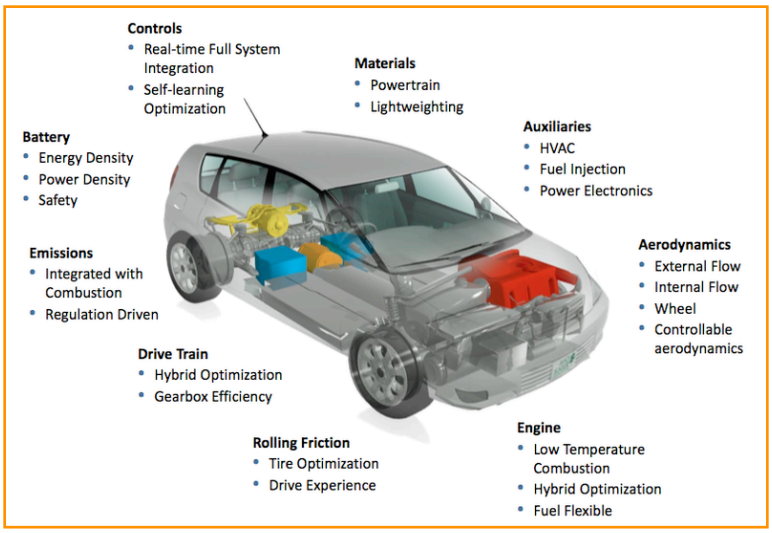
Inaugural Release of G-IncSVD

Chris Baker (CSMD) recently performed the inaugural release of a G-IncSVD, an incremental algorithm for computing dominant singular subspaces on NVIDIA CUDA-capable graphics processing units (GPUs). This algorithm is useful for performing streaming analysis and compression of large data sets. This software release joins previous software releases in this project, including a MATLAB software package and high-performance implementation in the Trilinos project. The algorithm is described in a recent journal publication, "Low-Rank Incremental Methods for Computing Dominant Singular Subspaces", in Linear Algebra and Its Applications, with K. Gallivan (Florida State) and P. Van Dooren (UC-Louvain). Project pages (including software releases) are available from http://www.cgbaker.net/

High Performance Computing Key Enabler for Accelerating Development of High Efficiency Engines

Wael Elwasif, Srdjan Simunovic, Miro Stoyanov, Clayton Webster and Sreekanth Pannala from CSMD; Robert Wagner, Dean Edwards, Charles Finney and Stuart Daw from ETSD
Green Car Congress - 5 November 2012

The complexity of new and future vehicles—driven by the need for increasing fuel efficiency and decreasing emissions with ever-changing drive-cycle demands and environmental conditions—is adding unprecedented flexibility in design and driving the need for better simulation and more powerful computers, observed Dr. Robert M. Wagner, Director of the Fuels Engines and Emissions Research Center, and Dr. Sreekanth Pannala, Senior Research Staff Member in the Computing and Computational Sciences Directorate at Oak Ridge National Laboratory in a keynote talk at the recent Global Powertrain Conference.
Advances in high performance computing (HPC) resources are leading to a new frontier in engine and vehicle development, Wagner and Pannala suggested, including the ability to produce detailed simulations to generate benchmark data; engineering simulations to explore the design space (e.g., injector optimization at ORNL); and reduced models for design optimization and control strategies. In general, HPC can help solve problems which were once thought unsolvable, they noted.
Click HERE to read more.



Increasing complexity of vehicle design is driving the need for better simulation and more powerful computers. Wagner and Pannala.

Ongoing Work

Cheetah: A Framework for Collective Communications for Heterogeneous Network Systems

DOE FastOS Program

To meet the needs of scientific simulations, supercomputers speeds are growing at a relentless pace. Earlier massively parallel computers had compute nodes consisting of a small number of processors – typically just one or two. However with the rise of multi-core processors, today's systems often have up to one or two dozen processor cores per node. Further, today's systems often have multiple communications mechanisms available with different performance and scalability characteristics. Unfortunately, the implementations of collective communication operations have not kept pace with these changes. Collective operations are used in parallel computing to synchronize processes, and for other operations in which all processes participate, such as broadcasts and reductions. Collective operations are often among the most sensitive parts of scientific simulations with regard to performance and scalability. Unfortunately, collective operations which have been designed for supercomputers with single- or dual-processor nodes and a particular network fabric can become scalability and performance bottlenecks on today's many-core compute nodes, and when used on different network fabrics.

Cheetah, a framework for implementing collective operations, was built ground up to address these problems. The goal of Cheetah is to provide an efficient collective operations implementation for modern supercomputers, and for various programming models including message passing and global address space models. Cheetah achieves this goal by designing the collective operation as a combination of simple collective primitives, which are each optimized for a different homogeneous block in the heterogeneous architecture. In addition, also by enabling asynchronous progress, computation can be progressed in parallel along with the communication, and enabling communication offload to network hardware, so computation can be overlapped with the communication.

Cheetah was a joint effort of Oak Ridge National Laboratory (ORNL), and Mellanox Technologies. The Cheetah research shaped the features and capabilities of Mellanox's CORE-Direct technology, which is now a part of their products. The ORNL team includes Pavel Shamis and Manjunath Gorentla Venkata, who are both members of Computer Science Research Group. They, along with researchers and engineers from Mellanox Technologies, built many prototypes before arriving at the current solution.

Cheetah 1.0.0, the first version to be officially released, will appear in forthcoming releases of Open MPI, a widely-used open source implementation of the MPI-2 standard, and is already available to Open MPI developers. This release includes the infrastructure to implement collectives, and reference implementations of the barrier and broadcast collective operations. The reference implementation outperforms the native implementations on Cray XE/XK and InfiniBand systems, and scales to over 100,000 cores on Cray XE/XK systems. The scalability and performance results of Cheetah on various architectures are published in over 12 peer-reviewed conference and workshop publications.

A complete list of contributors and details of this project are available at the project website: http://www.csm.ornl.gov/cheetah/

Abstract Scalable Performance Engineering Notation (Aspen)

DARPA UHPC Echelon, DOE Co-design ExMatEx

Aspen is a domain specific language for performance modeling that fills an important gap in existing techniques for performance prediction. It is designed to enable rapid exploration of new algorithms and architectures. It includes a formal specification of an application's performance behavior and an abstract machine model. It also includes a suite of analysis tools that operate on these models to provide valuable insights for the co-design process. ORNL's Future Technologies group will present Aspen and its use in modeling a three dimensional Fast Fourier Transform at this year's International Conference for High Performance Computing, Networking, Storage, and Analysis (SC '12).

Scalable HeterOgeneous Computing (SHOC)

NSF Keeneland, DOE X-Stack Vancouver

ORNL's Future Technologies group has released several updates to the SHOC benchmark suite. SHOC contains performance and stability tests for systems with accelerators such as graphics processing units using both CUDA and OpenCL. SHOC has enjoyed widespread adoption, including use in system procurements as well as regression tests at major hardware vendors including NVIDIA and Intel. The current version (v1.1.4) includes ease of use improvements, performance optimizations, and bug fixes (see http:/bit.ly/shocmarx).

Multigrid Algorithm for K-Version Finite Element Method

ORNL SEED Money

Rahul Sampath (PI) and Srikanth Allu (co-investigator)

In this project, the researchers have developed a new framework to solve partial differential equations (PDEs) efficiently. First, they discretize the PDEs using a recently developed numerical technique known as k-version Finite Element Method (K-FEM) that results in higher-order accuracy. The focus of this project was the second component – a new multigrid algorithm to solve the resulting system of linear equations. The higher-order accurate discretizations result in smaller systems of linear equations as compared to standard techniques and the multigrid algorithm enables the solution of these systems of equations with nearly optimal complexity. When tested on a model PDE, the new framework reduced the error in the solution by over a factor of 3 and reduced the time taken to solve the PDE by a factor of 30 as compared to the standard technique.

LDRD Projects

A Hierarchical Regional Modeling Framework for Decadal-scale Hydro-Climatic Predictions and Impact Assessments

Team Members: Moetasim Ashfaq (PI), Shih-Chieh Kao, Abdoul Oubeidillah, Rui Mei, Danielle Touma, Syeda Absar, Valentine Anantharaj

Probabilistic prediction of climate change at decadal-scale, and quantification of its impacts on natural and human systems is a great scientific challenge, and one that has significant potential to inform decision-making regarding the management of climate risk. Due to their policy relevance, 8-10 global modeling groups will undertake decadal-scale prediction experiments of the global climate as part of the Fifth Coupled Model Inter-comparison Project (CMIP5), whose results will be an integral part of the Fifth Assessment Report of the International Panel on Climate Change (IPCC-AR5). While a new generation of General Circulation Models (GCMs) has improved substantially in the simulation of the large-scale response to climate forcing, GCM resolution and accuracy is still inadequate to fully understand the response of regional-to-local-scale processes, particularly those governing hydro-climatic extremes. To improve on the limitations of GCMs, we will develop a hierarchical regional modeling framework to substantially enhance our ability in the quantitative understanding of the decadal-scale climate change at national and sub-national levels, and its potential implications for energy, water resources, and other sectors. This framework will use a suite of Earth system models and statistical techniques to downscale predictions from a multi-model ensemble of IPCC-AR5 global models to an ultra-high horizontal resolution of 4 km over the United States and South Asia.

Integrated Computational Modeling and Innovative Processing to Eliminate Rare Earths from Wrought Magnesium Alloys

ORNL Team Members: Balasubramaniam Radhakrishnan, Zhili Feng, Ryan Dehoff, Sarma Gorti, Robert Patton, William Peter, Amit Shyam and Srdjan Simunovic

Project Description: The project seeks to integrate micromechanical material models, process models and experimental data through a multi-objective optimization tool to design a microstructure that optimizes two conflicting material properties. The integrated approach addresses a critical need in the microstructural design of structural materials for vehicle applications where conflicting properties have to be optimized, and provides the necessary framework to enable innovation in processing and the exploration of new micro-mechanical concepts. The integrated approach will be used to develop a rare earth free wrought magnesium alloy that meets or exceeds the current specifications in rare earth containing alloys for strength and ductility. The approach will target three innovative processes - friction stir extrusion, ultrasonic roll bonding and additive roll bonding to introduce mechanical alloying of magnesium with titanium to provide additional twin and slip systems in the alloy in the ultra-fine grain size range. Mechanical alloying will offer the potential to utilize nanotwins as structural barriers to dislocation flow as well as to allow glide of dislocations at the twin-matrix interface - a novel concept that has demonstrated simultaneous increase in strength and ductility in ultra fine grained copper.

Results and Accomplishments: An initial benchmark problem was defined that relates material microstructure and two different attributes of the microstructure, grain orientation and grain misorientation distribution, and couples with a genetic algorithm to optimize the two attributes. The problem was successfully solved. The problem was then extended to a coupling between a material micro-mechanics code that defines two material properties, strength and ductility as a function of the above microstructural attributes with a genetic algorithm. The two codes were run in parallel and an optimization of the strength and ductility was demonstrated. The optimization approach is being extended to other optimization methods that exist in the computational tool kit DAKOTA. Methods have also been developed to represent the input texture for optimization studies using orientation distribution functions that describe strong basal texture and weak basal texture in magnesium alloys. The crystal plasticity code used for the property computations has been extended to AZ31 alloy incorporating additional twin and slip systems as demonstrated in previous mechanical alloying studies of Ti with Mg. An additional glide system along the twin-matrix interface has also been introduced in order to study the influence of slip along the twin-matrix interface on the strength and ductility of AZ31. On the experimental side, a number of severe deformation processing experiments were attempted in order to demonstrate mechanical alloying of Ti with Mg/AZ31 alloy. The friction stir processing (FSP) approach showed a clear demonstration of Ti solubility in AZ31 and has been selected as the process of choice moving forward.

LDRD Projects (continued)

A Novel Uncertainty Quantification Paradigm for Enabling Massively Scalable Predictions of Complex Stochastic Simulations

ORNL Team Members: Chris Baker, Tom Evans and Clayton Webster (PI)

We propose a transformational methodology related to the efficient, accurate and robust computation of statistical quantities of interest (QoIs), i.e., the information used by engineers and decision makers, that are determined from solutions of complex stochastic simulations. Our objective is to effect a transition from current stochastic polynomial approximation techniques, which lack the ability to easily harness powerful high-performance computing (HPC) architectures, to a truly predictive science. That is, to develop an innovative approach for uncertainty quantification (UQ) that provides quantitative bounds on the applicability of extreme scale calculations. This remains a fundamental difficulty in most applications that dominate the focus of the DOE mission. Guided by this grand challenge in UQ, we propose a rigorous mathematical procedure for exploiting multicore extreme parallelism by simultaneously propagating numerous realizations of a multi-dimensional multi-resolution adaptive sparse grid stochastic collocation approach, through both the complex physics and the solver stack in a novel semi-intrusive fashion. This paradigm builds on existing progress in generic programming to selectively couple ensembles of the hierarchical decomposition while enabling advanced recycling and block solver techniques. This massively scalable UQ framework will be made available through a recently developed ORNL Toolkit for Adaptive Stochastic Modeling and Non-Intrusive ApproximatioN (TASMANIAN) and will be demonstrated by quantifying a moderately large number of uncertainties in a radiation transport calculation using the highly visible ORNL Denovo neutronics code.

Model-Inspired Science Priorities for Evaluating Tropical Ecosystem Response to Climate Change

ORNL team members: Forrest Hoffman (PI), Richard Norby, Xiaojuan Yang, Lianhong Gu, David Weston, and Jitendra Kumar

Carbon cycling in tropical forests and the feedbacks from tropical ecosystems to the climate system are critical uncertainties in current-generation Earth System Models (ESMs) that must be resolved to more reliably project global responses to climate change. The objectives of this ORNL Laboratory Directors' Research and Development (LDRD) project are to provide model improvements and initial model experiments and analyses that define the critical science objectives for a future planned DOE Next Generation Ecosystem Experiments (NGEE) project focused on tropical ecosystems and to provide guidance for an intensive campaign of structured observations and manipulative experiments. Leaf gas exchange measurements of tropical plant species, being performed at the Smithsonian Tropical Research Institute (STRI) in Panama, will drive improvements in how ESMs represent photosynthesis and phosphorus limitations to carbon cycling. Model improvements based on these data will be implemented into the Community Land Model (CLM4), and experiments using the improved model will define the relative sensitivity of tropical forests to elevated carbon dioxide, climate warming, and drought. Cluster analysis that combines current-generation models with large-scale climate and geophysical observations will provide quantitative delineation of tropical regions that are most important for intensive observations and modeling. Together, these model products will guide the development of an experimental framework, define critical field experiments, and initiate the iterative process of model-experiment interaction.

Toward Scalable Algorithms for Kinetic Equations: A New Hybrid Approach to Capturing Multiscale Phenomena

ORNL team members: Cory Hauck, Yulong Xing, and Jun Jia

The goal of this LDRD project is to design and implement a hybrid method for the efficient solution of multi-scale kinetic equations, which play a fundamental role in many areas of mathematical physics. Kinetic models are mesoscopic: on one hand, they provide a detailed and accurate description of particle-based systems in regimes where traditional fluid dynamic models are either invalid or simply not available. On the other hand, they can incorporate important features from a molecular- or quantum-level description that cannot be modeled directly because of the prohibitive computational cost. Consequently, kinetic models are an indispensable tool in the mathematical description of gas dynamics, plasma physics, multiphase flow, and radiative transport - all key components of current and future energy generation systems. Moreover, in recent years, kinetic theory has emerged as an important analytical tool in other important applications, including traffic and network models, computational biology and chemistry, and self-organization of complex systems. Even with exascale resources, the full resolution of all dynamical scales in a kinetic equation is generally not possible. Rather, a robust simulation capability will only be achieved through the advent of new numerical methods that exploit the mathematical structure in the equations. In particular, details of mesoscopic processes that do not affect macroscopic behavior can be approximated by reduced

models with significant savings, both in floating point operations and in memory storage and transfer. The mathematical challenge is how to derive these models and incorporate them into a rigorous mathematical framework that guarantees accurate solutions. The proposed hybrid methods involves an intelligent separation of the kinetic equation based on dynamical scales; a closure method for approximation of functions using limited data; modern, low-memory, high-order discretization techniques; and implementation on GPUs. The resulting algorithms will be useful for a variety of application specialists, particularly in high performance computing environments.

A Comprehensive Theoretical/Numerical Tool for Electron Transport in Mesoscale-Heterostructures

ORNL team members: Xiaoguang Zhang (PI), Mina Yoon, An-Ping Li, Don Nicholson

Modeling electron transport in electronic devices using macroscopic equations is a mature industry that generates billions of dollars per year. First-principles, quantum-mechanical modeling of atomic-scale transport has seen significant progress over the past decade. We identify a gap between these two length scales - the mesoscale, where effects described by macroscopic equations are dominant only in nanoscale devices because they depend on some power of a characteristic device length. One such phenomenon is space charge limited currents (SCLCs), a central feature of energy-related devices such as light-emitting diodes and organic solar cells, which entail carrier injection. A critical voltage for the onset of injection is proportional to the square of the device length. State-of-the-art commercial modeling tools do not treat such phenomena adequately. In particular, the available theory of SCLCs in the presence of traps either neglects or treats phenomelogically key physical effects such as the interplay between dopants and traps, the Frenkel effect, inter-trap tunneling (relevant at high trap concentrations), etc. Our goal is to develop a set of comprehensive simulation tools for modeling mesoscopic electronic devices that exhibit a strong SCLC effect, in particular quasi-zero, one, or two-dimensional structures, based on rigorous physics formulations of the pertinent problems. Such a toolset will provide a flexible foundation to build future energy research programs, e.g., battery modeling where charge carriers are ions, and is likely to attract industry interest.

Hardware/Software Resilience Co-Design Tools for Extreme-scale High-Performance Computing

ORNL team members: Christian Engelman (PI) and Thomas Naughton

The path to exascale computing poses several research challenges related to power, performance, resilience, productivity, programmability, data movement, and data management. Resilience, i.e., providing efficiency and correctness in the presence of faults, is one of the most important exascale computer science challenges as systems scale up in component count (100,000-1,000,000 nodes with 1,000-10,000 cores per node by 2020) and component reliability decreases (7 nm technology with near-threshold voltage operation by 2020). Several high-performance computing (HPC) resilience technologies have been developed. However, there are currently no tools, methods, and metrics to compare them and to identify the cost/benefit trade-off between the key system design factors: performance, resilience, and power consumption. This work focuses on developing a resilience co-design toolkit with definitions, metrics, and methods to evaluate the cost/benefit trade-off of resilience solutions, identify hardware/software resilience properties, and coordinate interfaces/responsibilities of individual hardware/software components. The primary goal of this project is to provide the tools and data needed by HPC vendors to decide on future architectures and to enable direct feedback to HPC vendors on emerging resilience threats.

Stochastic Parameterization of the Influence of Subgrid Scale Land Heterogeneity on Convection in a Climate Model

ORNL team members: Richard Archibald, Salil Mahajan, Jiafu Mao, Ben Mayer, Daniel S. McKenna (PI), Dan Ricciuto, Xiaoying Shi, Clayton Webster.

The convective parameterization in a climate model is a crucial component in the model climate system. State-of-the-science climate model simulations of precipitation tend to be too wide spread and to lack the intense episodes of precipitations found in observations. Our hypothesis is that model precipitation fails to capture to influence of small scale landscape heterogeneity and to a lesser extent dynamic surface variability. We propose to test this hypothesis and at the same time develop a stochastic parameterization of the surface fluxes that accounts for the influence of landscape heterogeneity. In the first stage of this project we will couple variants of the community land model (CLM) to the single column Community Land Model (SCAM) to create a basic

deterministic land atmosphere simulator and characterize this system. The by degrees we will introduce increasing degrees of stochastic parameterization by knowledge of landscape heterogeneity and dynamic variability. We will conduct initial sensitivity test by comparing column model simulations and where available high resolution regional simulations. Ultimately to goal is to introduce the stochastic parameterization into a fully 3-D version of CAM and test model sensitivity against regional precipitations statistics.

Improved Metagenomic Analysis with Confidence Quantification for Biosurveillance of Novel and Man-made Threats

ORNL team members: Chongle Pan (PI), Loren Hauser, Miriam Land, and Richard Stouder

Genetically engineered and naturally occurring, novel pathogens are currently blind spots of biosurveillance. Such threats confound or defeat standard biosurveillance techniques based on PCR and immunological assays. This challenge can be addressed by using a metagenomics approach, in which all microorganisms in a field sample are directly sequenced together. The genome of a pathogen, even if it is altered by natural recombination or genetic engineering, can be computationally reconstructed and identified from background microorganisms. The pathogen's genome provides information on its full malicious capability, evolutionary origin, and genetic manipulation history. Although next-generation sequencing technologies are ready for biosurveillance deployment, the informatics needed to extract information from the vast amount of sequencing data still requires significant improvements in terms of detection accuracy, analysis speed, and information content. The objective of this proposal is to develop an integrated informatics solution for applying metagenomics to accurately detect novel or man-made pathogens and comprehensively characterize their genetic capabilities in a short turnaround time. The key technical innovation of the proposed work is the construction of probabilistic error models of next-generation sequencing data and the quantification of statistical confidence in threat detection and characterization. The proposed informatics solution will be systematically tested and evaluated for different biosurveillance scenarios using real-world and simulated metagenomic data.

Towards a Resilient and Scalable Infrastructure for Big Data

ORNL Team Members: Brad Settlemyer (PI), Sarp Oral, David Dillow, and Feiyi Wang

Commercial data-intensive computing and simulation science have divergent requirements in a number of areas, but both share the need for a resilient and scalable infrastructure for extreme-scale I/O. To address the requirements for these key drivers for computing platforms before the end of the decade, we must conduct research on novel software/hardware architectures and establish our laboratory as a key contributor to the state of the art in distributed I/O systems to satisfy the performance, capacity, and resiliency requirements of the Big Data era. In this project, we propose initial research required to design and evaluate the scalable object storage infrastructure that addresses the fundamental issues present in any Big Data system -- resiliency and performance of I/O at scale. To this end, we propose the following research:

1. New asynchronous storage programming models and advanced storage scheduling schemes that improve scalability and performance, provide quality of service guarantees, and support both scientific analysis techniques and modern loosely-coupled analysis codes;
2. New data location and replication schemes that ensure data access is mapped to devices that perform the target workloads with high performance while also duplicating important data to durable media in a timely manner ensuring that data is available even when portions of the storage system are unavailable (e.g., due to outages or scheduled maintenance); and
3. An evaluation of techniques for constructing hierarchical storage systems composed of multiple media types including magnetic disk, tape, and emerging non-volatile memory technologies such as Flash and evaluating candidate architectures with diverse Big Data workloads.

New Faces in CSMD

Jong Youl Choi

Jong Youl Choi's main research interest is large-scale data analysis and mining to solve I/O problems in HPC computing environments. His primary role in the team (Scientific Data Group) is to work with two fusion projects and play a leading role in machine learning and data management in fusion science. More specifically, Jong is currently working on researching and development tasks for mining provenance data collected from large-scale and data-intensive fusion applications.

Rajeev Kumar

Rajeev Kumar's title is Research and Development Associate: Soft Materials Theory and Simulation

His current research interests include dynamics of polymers, self-assembly of charged and neutral polymers in the bulk and near interfaces. He'll be working on the modeling of soft matter (mainly polymers) in close collaboration with experimentalists and applied mathematicians.

Moving On

Dr. Sudharshan Vazhkudai

Dr. Sudharshan Vazhkudai was named Group Leader for the Technology Integration Group of the National Center for Computational Sciences (NCCS). Sudharshan succeeds Galen Shipman, who moved into a new role of Data Systems Architect in CSMD. Dr. Vazhkudai will be responsible for technical leadership of the TechInt group, which is charged with delivering new technologies into the Leadership Computing Facility (OLCF) and other projects at ORNL by identifying gaps in the computing technology in use at ORNL and working with the R&D community to find, harden, and deploy solutions. Their technology scope has included archival storage, parallel file systems, high-performance networking, data analysis and movement, and data management technologies. He received his Ph.D. in Computer Science from the University of Mississippi in 2003, where he received support through a Givens Fellow/Doctoral Fellowship from Argonne National Laboratory. Next, he joined ORNL where he focused on advancements to the Globus toolkit capabilities. As an active R&D staff member over the past 9 years, Dr. Vazhkudai also holds a Joint Faculty Appointment with UTK through their CEE Department and the Joint Institute for Computational Sciences.

Awards

Distinguished Employee Program

The Computing and Computational Sciences Directorate program is recognizing an employee from each division each month for distinguished contributions; the first awards were made in April, 2011.

October

Ross Bartlett served as release manager for the Limited Beta Release of the Virtual Environment for Reactor Applications (VERA) through the Radiation Safety Information Computational Center (RSICC). VERA is the simulation environment being developed for the Consortium for Advanced Simulation of Light-Water Reactors (CASL), the DOE Innovation Hub for Modeling & Simulation for Nuclear Energy. Although limited to current CASL partners, this is the first "official" release of VERA components, and is a precursor to wide deployment for use by industry, academia, and research institutions.

November

Clayton Webster joined the Computational Engineering & Energy Sciences group in CSMD in May of 2011 to develop the growing area of uncertainty quantification. FY12 proved to be an extremely productive year, in which Clayton produced 15 papers, a similar number of invited conference presentations, and organized or co-organized 6 symposia at international conferences (such as SIAM and SAMSI). In addition, he led or participated in 16 proposals, serving as Principal Investigator on six. Five of these have been funded, with 1 expected and 5 awaiting decisions.

This award particularly recognizes Clayton's active involvement in development of industrial partnerships, including GE Global Research, Caterpillar, United Technologies, Pratt & Whitney, and most recently Proctor & Gamble. The Caterpillar and P&G interactions have recently borne fruit, resulting in additional funding for the growing UQ activities at ORNL.

Other Awards/Recognition

Jeff Vetter was appointed as an ACM Distinguished Scientist Member

The Association for Computing Machinery (ACM) has appointed CSMD researcher and Group leader Jeff Vetter as a Distinguished Scientist Member. The Distinguished Member Grade recognizes those ACM members with at least 15 years of professional experience and 5 years of continuous Professional Membership who have achieved significant accomplishments or have made a significant impact on the computing field.

Xiaoguang Zhang is now a Fellow of the American Physical Society!

CSMD researcher Xiaoguang Zhang has been recognized as a Fellow of the American Physical Society for his pioneering work in the development and application of the scattering theory and computational methods to materials studies, in particular to the study of electron transport in magnetic tunnel junctions.

Clayton Webster to Serve as Editor

CSMD researcher Clayton Webster has accepted an invitation to join the editorial board of SIAM J. Numerical Analysis. SINUM is the premier numerical analysis journal with long history and tremendous impact on the field of computational science. Clayton becomes the first ORNL researcher to serve on the editorial board and is one of only four editors currently at a national laboratory.

ForWarn Wins the 2013 FLC Interagency Partnership Award

An ORNL team was a recipient (along with the USDA Forest Service, NASA's Stennis Space Center, and U.S. Geological Survey's EROS Data Center) of the prestigious Federal Laboratory Consortium (FLC) for Technology Transfer Interagency Partnership Award.

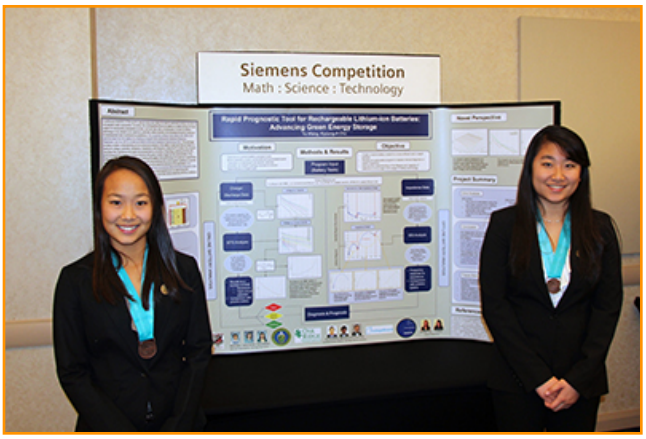
The ORNL team—comprised of Forrest Hoffman (ORNL PI), Jitendra "Jitu" Kumar, and Richard Tran Mills—contributed data mining methodologies for change detection to satellite remote sensing data. By analyzing the phenology in MODIS NDVI data over the continental US at a 250 m resolution, the team contributed to the Forest Service's ForWarn early warning system for

Awards (continued)

identifying threats to forest health. By working with researchers across four different federal agencies, the ORNL team were able to combine resources and expertise to meet a congressionally mandated mission for the Forest Service.

This award—one of the FLC's highest honors—recognizes the efforts of laboratory employees from at least two different agencies who have collaboratively accomplished outstanding work in the process of transferring a technology.

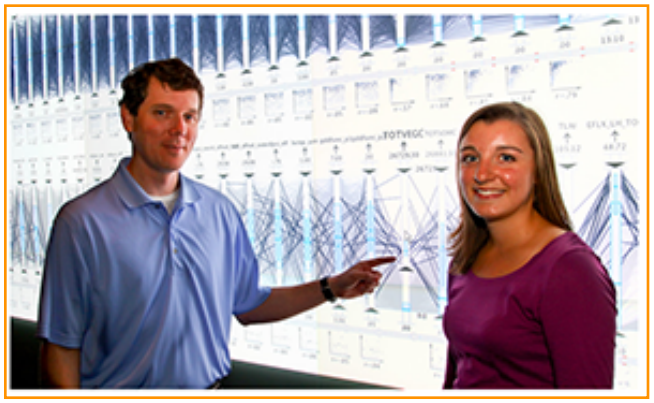
ORHS Students Shine in Regional Siemens Competition



Congratulations are in order for ORHS regional finalists Kyoung-A Cho and Samantha Wang, mentored by ORNL's Sreekanth Pannala, as well as semifinalists John Caughman III and Megan Kelly, mentored by the Lab's Blair Sullivan, and Patrick Williams, mentored by ORNL's Matthew Reuter.

The Siemens Competition in Math, Science & Technology recognizes remarkable talent early on, fostering individual growth for high school students who are willing to challenge themselves through science research. Through this competition, students have an opportunity to achieve national recognition for science research projects that they complete in high school.

FHS Student a Semifinalist in Intel competition



Alison Haugh, of Farragut High School, was a semifinalist in the Intel Science Talent search for 2013. Her work on "Decreasing the cost of high dimensional simulations of the community land model through machine learning and emulation" uses ideas from uncertainty quantification to provide tools to climate scientists to test and understand effects of model parameters with greater speed and accuracy. Alison Haugh, performed her senior math thesis project at the CCSI in the spring of 2012, and continued with her project over the summer and into the fall, dedication that produced results that impress the Intel Science Talent search committee.

Richard Archibald was Alison's mentor at the CCSI. Alison used the visualization tool EDEN (Exploratory Data analysis ENvironment) which is being developed under the DOE BER Climate Science for a Sustainable Energy Future (CSSEF) project. The data was generated by Peter Thornton and Dan Ricciuto (ORNL Environmental Sciences Division) on the CSSEF project. Chad Steed is a developer of EDEN and is in the picture showing Alison about the tool. Galen Shipman is also part of the collaborative team shaping the development of the EDEN.

CSMD Annual Awards

The 2012 award for the most distinguished Scientific Paper goes to Jingsong Huang and Bobby Sumpter for 'A Universal Model for Nanoporous Carbon Supercapacitors Applicable to Diverse Pore Regimes, Carbon Materials, and Electrolytes' published in the European Journal Chemistry (impact factor 5.925).

This paper provided breakthrough advances in the theory, modeling and simulation of nanoporous carbon-based supercapacitors. This work is the first demonstrated capability for the computer design and predictive simulation of high-capacity, cyclable, and versatile nanoporous supercapacitors for efficient and safe energy storage application. The papers has been cited on over 112 instances since 2008 and the journal publishers recognized its significance with a cover graphic.

Awards (continued)

The 2012 award for the most distinguished software release goes to N. Podhorszki, Q. Liu, Hassan. Abbasi, J. Choi, R. Tchoua and S. Klasky for the Adaptable IO System (ADIOS).

ADIOS provides a simple, flexible way for scientists to describe the data in their code that may need to be written, read, or processed outside of the running simulation. ADIOS routinely use over 300M core hours/year. Results that use the ADIOS framework have be published in over 80 computer science conferences/journals.

The 2012 special award for the most distinguished contribution goes to Ralf Deiterding for the release and support of the Adaptive Mesh Refinement in Object-oriented C++ (AMORC) Software.

AMORC is in use by many researchers and Ralf has personally supported the mesh refinement community by presenting extended tutorials at the Joint Institute for Computer Science and the 2010 Summer School on Multi-Resolution Methods, Frejus (France). The material from this summer school was also published in the European Series in Applied and Industrial Mathematics Proceedings. The code has been downloaded over 500 times.

The 2012 award for the most distinguished Scientific or Technical Contribution goes to Forrest Hoffman, Richard Mills and Jitendra (Jitu) Kumar for the ForWarn system.

ForWarn is a satellite-based monitoring and assessment tool that recognizes and tracks potential forest disturbances caused by insects, diseases, wildfires, extreme weather, or other natural or human-caused events. It is deployed operationally with the USDA Forest Service.

ForWarn is a partnership between ORNL, the USDA Forest Service, NASA's Stennis Space Center, and the U.S. Geological Survey's EROS Data Center and has been awarded the

- 2012 Southern Research Station Director's Award for Excellence in Science Delivery and the
- 2013 Federal Laboratory Consortium (FLC) for Technology Transfer Interagency Partnership Award

The ORNL ForWarn team - comprised of Forrest Hoffman (ORNL PI), Jitendra "Jitu" Kumar, and Richard Tran Mills - contributed data mining methodologies for change detection to satellite remote sensing data.

Events

Seminars

Russell Carden: Automating and Stabilizing the Discrete Empirical Interpolation Method for Nonlinear Model Reduction

Charlotte Kotas: Bringing Real-Time Array Signal Processing to the NVIDIA Tesla

Shuaiwen "Leon" Song: Power, Performance and Energy Models and Systems for Emergent Architectures

Miroslav Stoyanov: Gradient Based Dimension Reduction Approach for Stochastic Partial Differential Equations

Barbara Chapman: Enabling Exascale Programming: The Intranode Challenge

Andrew Christlieb: An Implicit Maxwell Solver Based on Method of Lines Transpose

Charles Jackson: Metrics for Climate Model Validation

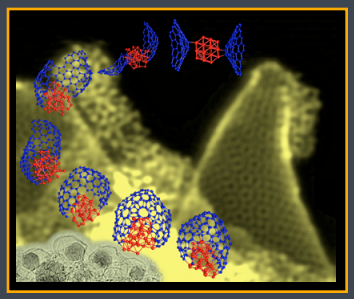
Erich Foster: Finite Elements for the Quasi-Geostrophic Equations of the Ocean

Shi Jin: Asymptotic-Preserving Schemes for Boltzmann Equation and Relative Problems with Stiff Sources

Shi Jin: Semiclassical Computation of High Frequency Waves in Heterogeneous Media

Christian Ringhofer: Charged Particle Transport in Narrow Geometries under Strong Confinement

Amilcare Porporato: Stochastic soil moisture dynamics: from soil-plant biogeochemistry and land-atmosphere interactions to sustainable use of soil and water



Cover Art

The process by which curved nanocones of carbon (blue) encapsulate Fe nanoparticles (red) to form a new hybrid "nanooyster" material (inset) is shown through snapshots of QM/MD simulations. Background is an aberration-corrected, atomic resolution, Z-STEM image of single wall carbon nanohorns and unconverted graphene flakes which served as the feedstock in the process.

The above image will appear on the cover of the journal *Nanoscale*.

Publications/Presentations

Journal Publications

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- Mahajan, Salil, et al. "Inter-annual Global Tropospheric Aerosol Variability and its Impacts on Atlantic and African Climate by Direct and Semi-direct Effects." 17th Annual CESM Workshop, Breckenridge, Colorado, USA, June 18, 2012.
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- Rudakov, Fedor M., et al. Ultrafast Structural Dynamics Probed by Photoionization and Microwave Rayleigh Scattering from Laser Induced Plasma. LDRD Report. Oak Ridge, TN: Oak Ridge National Laboratory.2012.
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- Shipman, Galen M., et al. 06349 - Accelerating Data Acquisition, Reduction, and Analysis (ADARA) at SNS. LDRD Report. Oak Ridge, TN: Oak Ridge National Laboratory.2012.
- Spafford, Kyle, and Vetter, Jeffrey S., Aspen: A Domain Specific Language for Performance Modeling. SC12: Proceedings of the 2012 ACM/IEEE conference on Supercomputing, November, 2012.
- Su, Chun-Yi, et al. "Model-Based, Memory-Centric Performance and Power Optimization on NUMA Multiprocessors." In International Symposium on Workload Characterization, 2012.
- Su, Chun-Yi, Li, Dong, Nikolopoulos, Dimitrios S., Cameron, Kirk W., de Supinski, Bronis R., Leon, Edgar A., "Model-Based, Memory-Centric Performance and Power Optimization on NUMA Multiprocessors". In International Symposium on Workload Characterization (IISWC), 2012
- Sullivan, Blair D., et al. "Finding a role for structural graph theory in real-world network analysis." 2012.
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Publications/Presentations (continued)

- Sun, Yanhua, et al. "A uGNI-Based Asynchronous Message-driven Runtime System for Cray Supercomputers with Gemini Interconnect." In 26th IEEE International Parallel & Distributed Processing Symposium (IEEE IPDPS 2012), 2012.
- Sun, Yanhua, et al. "Optimizing Fine-grained Communication in a Biomolecular Simulation Application on Cray XK6." In International Conference for High Performance Computing, Networking, Storage and Analysis (SC'12), 2012.
- Webster, Clayton G., et al. LDRD annual project summary. LDRD Report. Oak Ridge, TN: Oak Ridge National Laboratory. 2012.
- Webster, Clayton G., Guannan Zhang and Max D. Gunzburger. An adaptive wavelet stochastic collocation method for irregular solutions of stochastic partial differential equations. ORNL/TM-2012/186. Oak Ridge, TN: Oak Ridge National Laboratory.2012.
- Worley, Patrick H., et al. "Approaches to and Tools for Project Performance Tracking and Analysis." Scientific Discovery through Advanced Computing (SciDAC-3) Principal Inverstigator Meeting, Rockville, Maryland, USA, September 10—12, 2012.
- Yu, Li, et al. "Filtering log data: finding the needles in the haystack." In 42nd IEEE/IFIP International Conference on Dependable Systems and Networks (DSN 2012), 2012.
- Zhang, B., Lu, B., Cheng, X., Sun, X., Pitsianis, N., Huang, J., and McCammon, J.A., “Mathematical and numerical aspects of the adaptive fast multipole Poisson-Boltzmann solver”. Commun Comput Phys, 2013, 13(1), 107-128
- Zhang, Guannan, Clayton G. Webster and Max D. Gunzburger. An adaptive sparse-grid high-order stochastic collocation method for Bayesian inference in groundwater reactive transport modeling. ORNL/TM-2012/499. Oak Ridge, TN: Oak Ridge National Laboratory.2012.
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Invited Presentations

- Allu, Srikanth, et al. "Computational Framework for Modeling Multi-Physics Phenomena of Li-Ion Batteries across Various Hierarchies." ECS Prime Fall Meeting, 2012., Honolulu, Hawaii, USA, October 07—12, 2012.
- Beste, Ariana and A C. Buchanan III. "Lignin Model Pyrolysis: A Computational Approach." ACS Rocky Mountain Regional Meeting, Westminster, Colorado, USA, October 17, 2012.
- Beste, Ariana “Probing complex free-radical reaction pathways of lignin model compounds“; Frontiers in Biorefining: Chemicals and Products from Renewable Carbon, St. Simons Island, GA, October, 2012
- Billings, Jay Jay, et al. "NiCE Demonstration for MFIX team." 2012.
- Hauck, Cory D., et al. "A Collision-Based Hybrid Method for Linear Transport." Boltzmann Models in Kinetic Theory, Providence, Rhode Island, USA, November 07—11, 2012.
- Hauck, Cory D., et al. "High-order, Entropy-based Models for Linear Transport in Slab Geometries." Kinetic and Quantum Transport, Reunion Conference, Lake Arrowhead, California, USA, December 12—16, 2012.
- Jones, Terry R., et al. "HPC Colony - Unconstrained Performance @ Exascale." Exascale Research Conference, Arlington, Virginia, USA, October 01, 2012.
- Kent, P.R.C. "Lithium ion batteries: from practice to theory", Joint Physics and Chemistry Seminar, Wake Forest University, Winston-Salem, NC. 31 October 2012.
- Lee ,Seyong, and Vetter, Jeffrey S., Early Evaluation of Directive-Based GPU Programming Models for Productive Exascale Computing, paper presentation, SC12: Proceedings of the 2012 ACM/IEEE conference on Supercomputing, November, 2012.

Publications/Presentations (continued)

- Lee, Seyong, Early Evaluation of Directive-Based GPU Programming Models, invited talk, the first KIISE-KOCSEA HPC SIG Joint Workshop on High Performance and Throughput Computing, November, 2012.
- Li, Dong, Classifying Soft Error Vulnerabilities in Extreme-Scale Scientific Applications Using a Binary Instrumentation Tool. SC12 paper presentation.
- Meredith, Jeremy S., panelist in SC12 Scientific Application Performance in Heterogeneous Supercomputing Clusters birds-of-a-feather (BOF) session
- Meredith, Jeremy S., panelist in SC12 Visualization Frameworks for Multi-Core and Many-Core Architectures panel
- Reuter, Matthew G. "Experiment and Theory in Electron Transport Studies", Symposium for Professor Mark Ratner's 70th Birthday, Evanston, IL, December 2012.
- Spafford, Kyle, Aspen: A Domain Specific Language for Performance Modeling. SC12 Paper Presentation.
- Sumpter, Bobby G. "Computational Studies of Nanostructured Soft Matter and Multicomponent Materials For Energy Sciences", The Bredesen Center for Interdisciplinary Research and Graduate Education, University of Tennessee, October (2012)
- Sumpter, Bobby G., Kai Xiao, Mike Kilbey, "Interfacial Compatibilizers and Buffer Layers for High Efficiency Organic Photovoltaics", Materials Research Society Meeting, Boston, MA, November (2012)
- Vetter, Jeffrey S., Meredith, Jeremy, Spafford, Kyle, Roth, Philip C., SC12 Tutorial titled "Scalable Heterogeneous Computing on GPU Clusters"
- Vetter, Jeffrey S., Roth, Philip C., panelists in SC12 DARPA High Productivity Computing Systems (HPCS) birds-of-a-feather (BOF) session
- Vetter, J.S., "Vancouver – Unlocking the Potential of Scalable Heterogeneous Systems." DOE Exascale Research Conference, Arlington, 2012, http://exascaleresearch.labworks.org/oct2012/
- Webster, Clayton,"An adaptive sparse grid stochastic collocation method for uncertain turbulent systems" Department of Mathematics, University of Pittsburgh
- Webster, Clayton, "An overview of stochastic Galerkin and collocation methods for UQ and PDEs with random input data"Department of Nuclear Engineering, North Carolina State University
- Webster, Clayton, "An adaptive wavelet stochastic collocation method for irregular solutions of PDEs with random input data"Department of Mathematics, North Carolina State University
- Webster, Clayton, "An adaptive sparse-grid high-order stochastic collocation method for Bayesian inference in groundwater reactive transport modeling"Department of Scientific Computing , Florida State University
- Webster, Clayton, " A gradient-based sampling approach for stochastic dimension reduction of PDEs with random input data" Department of Mathematics, Auburn University
- Worley, Patrick H., Panel on Software Engineering, DOE Workshop on Next Generation Innovations in Climate Modeling, December, 2012.
- Worley, Patrick H., Panel on Computer Performance, DOE Workshop on Next Generation Innovations in Climate Modeling, December, 2012.

Community Service

David E. Bernholdt, Workshop on the Latest Advances in Scalable Algorithms for Large-Scale Systems (ScalA) 2012 Program Committee
David E. Bernholdt, Engineering with Computers reviewer
David E. Bernholdt, Computational Science and Discovery reviewer
David E. Bernholdt, DOE SBIR program reviewer
Michael J. Brim, IPDPS 2013 Program Committee
Christian Engelmann, IEEE Transactions on Parallel and Distributed Systems (TPDS) reviewer
Christian Engelmann, IEEE Transactions on Computers (TC) reviewer
Christian Engelmann, 21st Euromicro International Conference on Parallel, Distributed and network-based Processing (PDP) Program Committee
Christian Engelmann, 13th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid) Program Committee
Dong Li, program committee member of International Workshop on Programming Models and Applications for Multicores and Manycores
Philip C. Roth, vice chair of SC12 Awards
Philip C. Roth, member of SC12 posters committee
Philip C. Roth, member of SC12 Dissertation Research Showcase committee
Philip C. Roth, judge, ACM Student Research Competition held at SC12
Philip C. Roth, session chair, First International Data Intensive Scalable Computing Systems workshop (DISCS-2012), co-located with SC12
Philip C. Roth, steering committee member, Parallel Data Storage Workshop 2012 (PDSW 2012)
Jeffrey S. Vetter, co-chair of SC12 Technical Papers
Patrick H. Worley, member of SC12 Technical Papers committee
Patrick H. Worley, member of SC12 Best Paper and Best Student Paper committee
Patrick H. Worley, member of SC12 panel on “Careers in HPC”, part of the ``Experiencing HPC for Undergraduates” program

CSMD researchers Rick Archibald and Clayton Webster were invited by the International Journal of Computer Mathematics (IJCM) to act as editors of an upcoming special IJCM publication. This special publication will consist of papers that were presented at the workshop Uncertainty Quantification for High Performance Computing that was held at ORNL this past May. Rick, Clayton, and Pierre Gremaud (from SAMSI) co-organized this workshop.

SuperComputing 2012

Once again, CSMD researchers played a substantial role in annual SuperComputing Conference. The following is a list of the Workshops, Tutorials, BOFs, and Paper sessions in which CSMD’s researchers took part.

Vassil Alexandrov, **Jack Dongarra, Al Geist, Christian Engelmann** - Workshop: 3rd Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems - ScalA

Novel scalable scientific algorithms are needed to enable key science applications to exploit the computational power of large-scale systems. This is especially true for the current tier of leading petascale machines and the road to exascale computing as HPC systems continue to scale up in compute node and processor core count. These extreme-scale systems require novel scientific algorithms to hide network and memory latency, have very high computation/communication overlap, have minimal communication, and have no synchronization points. Scientific algorithms for multi-petaflop and exa-flop systems also need to be fault tolerant and fault resilient, since the probability of faults increases with scale. With the advent of heterogeneous compute nodes that employ standard processors and GPGPUs, scientific algorithms need to match these architectures to extract the most performance. Key science applications require novel mathematical models and system software that address the scalability and resilience challenges of current and future-generation extreme-scale HPC systems.

Community Service (continued)

Jeffrey Vetter, Allen Malony, **Philip Roth, Kyle Spafford, Jeremy Meredith** - Tutorial: Scalable Heterogeneous Computing on GPU Clusters

This tutorial is suitable for attendees with an intermediate-level in parallel programing in MPI, and with some background in GPU programming in CUDA or OpenCL; it will provide a comprehensive overview on the optimization techniques to port, analyze, and accelerate applications on scalable heterogeneous computing systems using MPI and OpenCL, CUDA, and directive-based compilers using OpenACC. First, we will review our methodology and software environment for successfully identifying and selecting portions of applications to accelerate with a GPU, motivated with several application case studies. Second, we will present an overview of several performance and correctness tools, which provide performance measurement, profiling, and tracing information about applications running on these systems. Third, we will present a set of best practices for optimizing these applications: GPU and NUMA optimization techniques, optimizing interactions between MPI and GPU programming models. A hands-on session will be conducted on the NSF Keeneland System, after each part to give participants the opportunity to investigate techniques and performance optimizations on such a system. Existing tutorial codes and benchmark suites will be provided to facilitate individual discovery. Additionally, participants may bring and work on their own applications.

Nathan D. Fabian, Andrew C. Bauer, **Norbert Podhorszki**, Ron A. Oldfield, Utkarsh Ayachit - Tutorial: In-Situ Visualization with Catalyst

In-situ visualization is a term for running a solver in tandem with visualization. Catalyst is the new name for ParaView's coprocessing library. ParaView is a powerful open-source turnkey application for analyzing and visualizing large data sets in parallel. By coupling these together, we can utilize HPC platforms for analysis while circumventing bottlenecks associated with storing and retrieving data in disk storage. We demonstrate two methods for in-situ visualization using Catalyst. The first is linking Catalyst directly with simulation codes. It simplifies integration with the codes by providing a programmatic interface to algorithms in ParaView. Attendees will learn how to build pipelines for Catalyst, how the API is structured, how to bind it to C, C++, Fortran, and Python and how to build Catalyst for HPC architectures. The second method uses a variety of techniques, known as data staging or in-transit visualization, that involve passing the data through the network to a second running job. Data analysis applications, written using Catalyst, can operate on this networked data from within this second job minimizing interference with the simulation but also avoiding disk I/O. Attendees will learn three methods of handling this procedure as well as the APIs for ADIOS and NESSIE.

Cyrus Harrison, Jean M. Favre, Hank Childs, **Dave Pugmire**, Brad Whitlock, Harinarayan Krishnan - Tutorial: Large Scale Visualization and Data Analysis with VisIt

This full-day tutorial will provide attendees with a practical introduction to VisIt, an open source scientific visualization and data analysis application. VisIt is used to visualize simulation results on wide range of platforms from laptops to many of the world's top supercomputers. This tutorial builds on the success of past VisIt tutorials with material updated to showcase the newest features and use cases of VisIt. We will show how VisIt supports five important scientific visualization scenarios: data exploration, quantitative analysis, comparative analysis, visual debugging, and communication of results. We begin with a foundation in basic principles and transition into several special topics and intermediate-level challenges. The last portion of the tutorial will discuss advanced VisIt usage and development, including writing new database readers, writing new operators, and how to couple VisIt with simulations executing on remote computers for in-situ visualization.

Jack Dongarra, James Demmel, Michael Heroux, Jakub Kurzak - Tutorial: Linear Algebra Libraries for High-Performance Computing: Scientific Computing with Multicore and Accelerators

Today, a desktops with a multicore processor and a GPU accelerator can already provide a TeraFlop/s of performance, while the performance of the high-end systems, based on multicores and accelerators, is already measured in PetaFlop/s. This tremendous computational power can only be fully utilized with the appropriate software infrastructure, both at the low end (desktop, server) and at the high end (supercomputer installation). Most often a major part of the computational effort in scientific and engineering computing goes in solving linear algebra subproblems. After providing a historical overview of legacy software packages, the

tutorial surveys the current state-of-the-art numerical libraries for solving problems in linear algebra, both dense and sparse. PLASMA, MAGMA and Trilinos software packages are discussed in detail. The tutorial also highlights recent advances in algorithms that minimize communication, i.e. data motion, which is much more expensive than arithmetic.

Ranga Raju Vatsavai, Scott Klasky, Manish Parashar, Hasan Abbasi - Workshop: 3rd SC Workshop on Petascale Data Analytics: Challenges and Opportunities
Recent decade has witnessed data explosion, and petabyte sized data archives are not uncommon any more. It is estimated that organizations with high end computing (HEC) infrastructures and data centers are doubling the amount of data that they are archiving every year. On the other hand computing infrastructures are becoming more heterogeneous. The first two workshops held with SC-2010 and SC-2011 are a great success. Continuing on this success, in addition to the cloud focus, we propose to broaden the topic of this workshop with an emphasis on middleware infrastructure that facilitate efficient data analytics on big data. The proposed workshop intends to bring together researchers, developers, and practitioners from academia, government, and industry to discuss new and emerging trends in high end computing platforms, programming models, middleware and software services, and outline the data mining and knowledge discovery approaches that can efficiently exploit this modern computing infrastructure.

Bing Xie, Jeff Chase, David Dillow, Oleg Drokin, **Scott Klasky**, Sarp Oral, **Norbert Podhorszki** - Papers: Characterizing Output Bottlenecks in a Supercomputer
Supercomputer I/O loads are often dominated by writes. HPC (High Performance Computing) file systems are designed to absorb these bursty outputs at high bandwidth through massive parallelism. However, the delivered write bandwidth often falls well below the peak. This paper characterizes the data absorption behavior of a center-wide shared Lustre parallel file system on the Jaguar supercomputer. We use a statistical methodology to address the challenges of accurately measuring a shared machine under production load and to obtain the distribution of bandwidth across samples of compute nodes, storage targets, and time intervals. We observe and quantify limitations from competing traffic, contention on storage servers and I/O routers, concurrency limitations in the client compute node operating systems, and the impact of variance(stragglers) on coupled output such as striping. We then examine the implications of our results for application performance and the design of I/O middleware systems on shared supercomputers.

Seyong Lee, **Jeffrey S. Vetter** and Michael A. Heroux - Papers: Early Evaluation of Directive-Based GPU Programming Models for Productive Exascale Computing
Graphics Processing Unit (GPU)-based parallel computer architectures have shown increased popularity as a building block for high performance computing, and possibly for future Exascale computing. However, their programming complexity remains as a major hurdle for their widespread adoption. To provide better abstractions for programming GPU architectures, researchers and vendors have proposed several directive-based GPU programming models. These directive-based models provide different levels of abstraction, and required different levels of programming effort to port and optimize applications. Understanding these differences among these new models provides valuable insights on their applicability and performance potential. In this paper, we evaluate existing directive-based models by porting thirteen application kernels from various scientific domains to use CUDA GPUs, which, in turn, allows us to identify important issues in the functionality, scalability, tunability, and debuggability of the existing models. Our evaluation shows that directive-based models can achieve reasonable performance, compared to hand-written GPU codes.

Tingxing Dong, Tzanio Kolev, Robert Rieben, Veselin Dobrev, Stanimire Tomov, **Jack Dongarra** - Posters: Acceleration of the BLAST Hydro Code on GPU
The BLAST code implements a high-order numerical algorithm that solves the equations of compressible hydrodynamics using the Finite Element Method in a moving Lagrangian frame. BLAST is coded in C++ and parallelized by MPI. We accelerated the most

computational intensive parts (80\%--95\%) of BLAST on NVIDIA GPUs with the CUDA programming model. Several 2D and 3D problems were tested and achieved an overall speedup of 4.3 on 1 M2050.

Stephen Poole, Bruce Childers - Birds of a Feather: Architecture and Systems Simulators
The goal of this BOF is to engage academia, government and industry to make sure that there is an open framework allowing interoperability of simulation tools for Computer Architecture. It is important to bring together and build a community of researchers and implementers of architecture simulation, emulation, and modeling tools. This BOF will inform Supercomputing attendees and solicit their involvement and feedback in an effort to build an interoperable, robust, community-supported simulation and emulation infrastructure.

Scott Klasky, Hasan Abbasi - Birds of a Feather: The Way Forward: Addressing the data challenges for Exascale Computing
This BOF will bring together application scientists, middleware researchers, and analysis and visualization experts to discuss the major challenges in the coordinated development of new techniques to meet the demands of exascale computing. In situ and in transit computations in a data pipeline has been proposed as an important abstraction in the next generation of I/O systems. We intend to explore the impact of this paradigm on algorithms and applications, as well as the evolution of middleware to achieve these goals.

Kyle L. Spafford, Jeffrey S. Vetter - Papers: Aspen - A Domain Specific Language for Performance Modeling
We present a new approach to analytical performance modeling using Aspen, a domain specific language. Aspen (Abstract Scalable Performance Engineering Notation) fills an important gap in existing performance modeling techniques and is designed to enable rapid exploration of new algorithms and architectures. It includes a formal specification of an application's performance behavior and an abstract machine model. We provide an overview of Aspen's features and demonstrate how it can be used to express a performance model for a three dimensional Fast Fourier Transform. We then demonstrate the composability and modularity of Aspen by importing and reusing the FFT model in a molecular dynamics model. We have also created a number of tools that allow scientists to balance application and system factors quickly and accurately.

Steve Poole, Tony Curtis - Birds of a Feather: OpenSHMEM: A standardized SHMEM for the PGAS community
The purpose of this meeting is to engage collaboration and input from users and developers of systems, libraries, and applications to further expand an open organization and specification for OpenSHMEM. The initial specification is based on the existing SGI API, but we are now discussing concrete ideas for extensions and expect more to come as this new API is ported to a large variety of platforms. We will also talk about other PGAS frameworks and their relationship with OpenSHMEM, plus the OpenSHMEM "ecosystem" of implementations, applications and tool support.

Janine C. Bennett, **Hasan Abbasi**, Peer-Timo Bremer, Ray W. Grout, Attila Gyulassy, Tong Jin, **Scott Klasky**, Hemanth Kolla, Manish Parashar, Valerio Pascucci, Philippe Pébay, David Thompson, Hongfeng Yu, Fan Zhang, Jacqueline Chen - Papers: Combining In-Situ and In-Transit Processing to Enable Extreme-Scale Scientific Analysis
With the onset of extreme-scale computing, scientists are increasingly unable to save sufficient raw simulation data to persistent storage. Consequently, the community is shifting away from a post-process centric data analysis pipeline to a combination of analysis performed in-situ (on primary compute resources) and in-transit (on secondary resources using asynchronous data transfers). In this paper we summarize algorithmic developments for three common analysis techniques: topological analysis, descriptive statistics, and visualization. We describe a resource scheduling system that supports various analysis workflows, and discuss our use of the DataSpaces and ADIOS frameworks to transfer data between in-situ and in-transit computations. We demonstrate the efficiency of our lightweight, flexible framework on the Jaguar XK6, analyzing data generated by S3D, a massively parallel turbulent combustion code. Our framework allows scientists dealing with the data deluge at extreme-scale to perform analyses at increased temporal resolutions, mitigate I/O costs, and significantly improve time to insight.

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 10 of Groups. These Groups and their Group Leaders are:

- Complex Systems - Jacob Barhen
- Computational Astrophysics - Tony Mezzacappa
- Computational Chemical and Materials Sciences - Bobby Sumpter
- Computational Earth Sciences - Danny McKenna
- Computational Engineering and Energy Sciences - John Turner
- Computational Mathematics - Ed D'Azevedo (Interim)
- Computer Science Research – David Bernholdt
- Future Technologies - Jeff Vetter
- Scientific Data - Scott Klasky

About this Newsletter

This newsletter is compiled from information submitted by CSMD Group Leaders, public announcements and searches.

Please contact Daniel Pack if you have information you would like to contribute.

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LINKS

Computer Science and Mathematics Division - www.csm.ornl.gov
Computing and Computational Sciences Directorate - computing.ornl.gov
Oak Ridge National Laboratory - www.ornl.gov

OAK RIDGE National Laboratory