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CSMD

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Science Highlights

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

Richard Archibald and Guannan Zhang

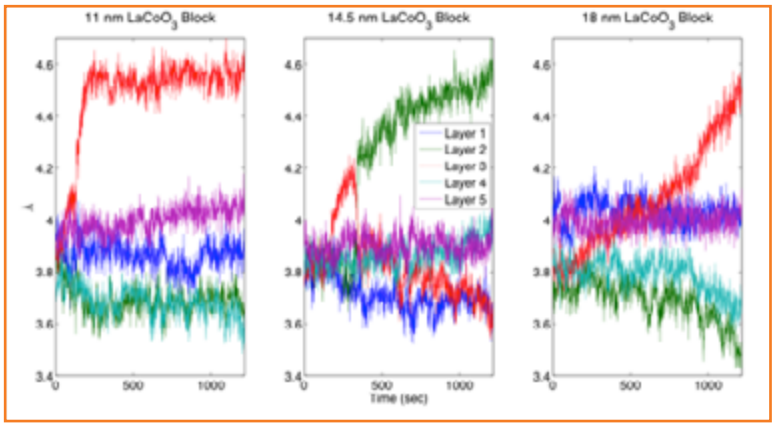
A multi-disciplinary team of scientist from across DOE laboratories and experimental facilities demonstrated the capability to merge resources and expertise to produce near real-time identification of oxygen migration in $LaCoO_3$. This understanding is key in identifying the electrical storage properties of $LaCoO_3$ for possible development of new battery technology.

The sophisticated neutron and computational science facilities at Oak Ridge National Laboratory (ORNL) are staffed by experts uniquely qualified to address the scientific, mathematical, and computational challenges encountered by key mission areas within the Department of Energy (DOE). The goal of this project is to develop innovative methods focused on core mathematical challenges that face neutron scientists and strengthen the existing integration of instrument scientists at both the Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFIR) with mathematicians at ORNL. This unified team will combine its solutions into a common framework for users at SNS and HFIR that we call ACUMEN – Accurate qUantified Mathematical mEthods for Neutron science.

This work was sponsored by Advanced Scientific Computing Research (ASCR): ACcurate qUantified Mathematical mEthods for Neutron science (ACUMEN).

Read the full document [**here**].

http://scdoe.info/2014/11/11/rick-archibald-oak-ridge/



Migration of layers for various thickness of $LaCoO_3$

OAK RIDGE National Laboratory

Science Highlights [Continued]

Omega: an Overlap-graph de novo Assembler for Metagenomics

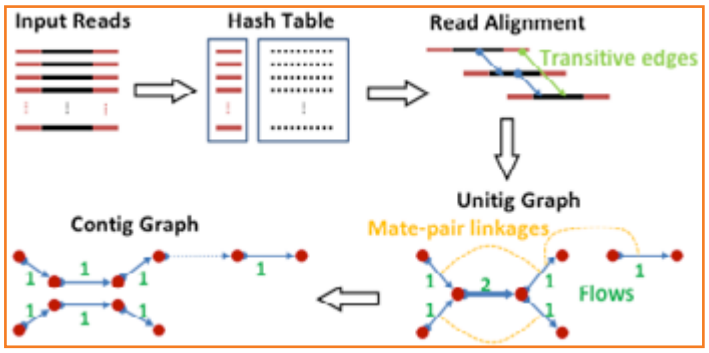
Chongle Pan

Metagenome assemblers attempt to reconstruct genomes of microorganisms in a community from its metagenomic sequencing data. Omega (over-lap-graph metagenome assembler) was developed for assembling and scaffolding Illumina sequencing data of microbial communities.

Omega provided comparable overall performance on a HiSeq 100-bp dataset and superior performance on a MiSeq 300-bp dataset. In comparison to Celera on the MiSeq dataset, Omega provided more continuous assemblies overall using a fraction of the computing time of existing Overlap-Layout-Consensus assemblers. This indicates Omega can more efficiently assemble longer Illumina reads, and at deeper coverage, for metagenomic datasets.

This work was supported by Laboratory Directed Research and Development (LDRD) funding from Oak Ridge National Laboratory and the Emerging Technologies Opportunity Program (ETOP) from DOE Joint Genome Institute.

Read more about Omega [**here**]. http://www.ncbi.nlm.nih.gov/pubmed/24947750



Overview of Omega. The prefix and suffix (red sections) of every read are indexed in a hash table. As reads are aligned using the hash table, transitive edges (green arrows) are removed. In the unitig graph, edges (blue arrows) represent unambiguous series of overlapping reads, vertices (red dots) represent branching points, and flows (green numbers) estimate the copy numbers of strings in the edges. The mate-pair linkages (orange dotted lines) are used to build contigs and then scaffolds containing gaps (blue dotted arrows). The repeat region between two different genomes (the edge with 2 units of flow) may be resolved using mate-pair supports (as shown here) or coverage depth information.

Sigma: Strain-level Inference of Genomes from Metagenomic Analysis for Biosurveillance

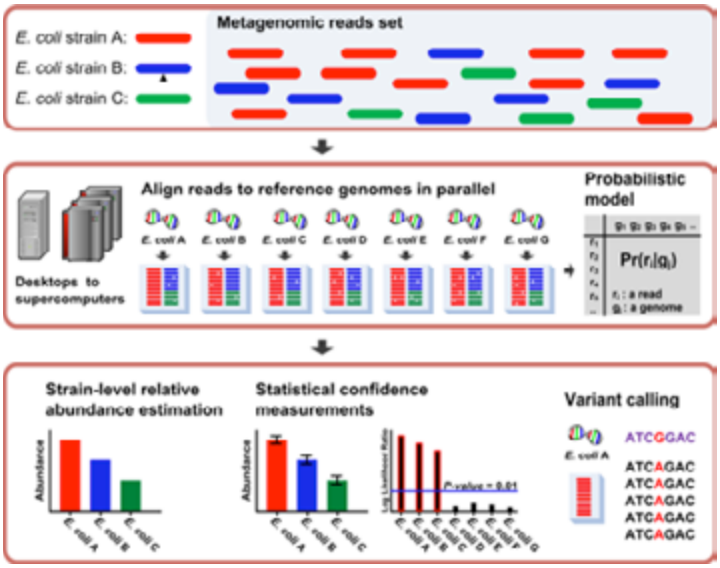
Chongle Pan

Metagenomic sequencing of clinical samples provides a promising technique for direct pathogen detection and characterization in biosurveillance. Taxonomic analysis at the strain level can be used to resolve serotypes of a pathogen in biosurveillance. Sigma was developed for strain-level identification and quantification of pathogens using their reference genomes based on metagenomic analysis.

Sigma has the unique capability of identifying the correct strain of a pathogen in a complex metagenomic background from many closely related candidates in the reference genome database. Using a top open-science supercomputer, Titan, pathogenic bacteria strains can be identified in an hour from the 100 million human microbiome sequences.

This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

Read more about Sigma [**here**]. http://www.ncbi.nlm.nih.gov/pubmed/25266224



Conceptual overview of the Sigma algorithm. The inputs are metagenomic reads and user-defined reference genomes (top panel). The alignment of reads to genomes is used to define a probabilistic model of metagenomic sequencing (middle panel). Genomes are detected with hypothesis testing, quantified with confidence interval estimation, and scanned for sequence variations (bottom panel).

Science Highlights [Continued]

A Gradient-bases Sampling Approach for Dimension Reduction of Partial Differential Equations with Stochastic Coefficients

Clayton Webster and Miroslav Stoyanov

We have developed an algorithm that identifies the active subspace form samples of the gradient of the QoI. We have proven that our method converges no worse than $O(k^{-1})$, independently from the number of inputs. We present, in Figure 1, numerical examples of linear and nonlinear equations that demonstrate that our convergence estimates are generally sharp, and in some cases we observe that a sufficiently accurate subspace can be formed form a sample set that is significantly smaller than what is predicted by the theoretical confidence estimates. Thus, when applied to problems with large number of input parameters, if the dynamics of a QoI are dominated by a low dimensional active subspace, our reduction approach is superior to brute force Monte Carlo.

Sampling based approaches, such as sparse grids (SG) and quasi-Monte Carlo (qMC) can exhibit rapid convergence when approximating the variation in response of partial differential equations due to random inputs. However, as the number of inputs increases, the efficiency of those methods quickly deteriorates. The brute force Monte Carlo (MC) method is the only direct approach applicable to problems with hundreds or thousands of uncertain parameters, and MC is associated with slow $O(k^{-1/2})$ rate of convergence (k is the number of samples).

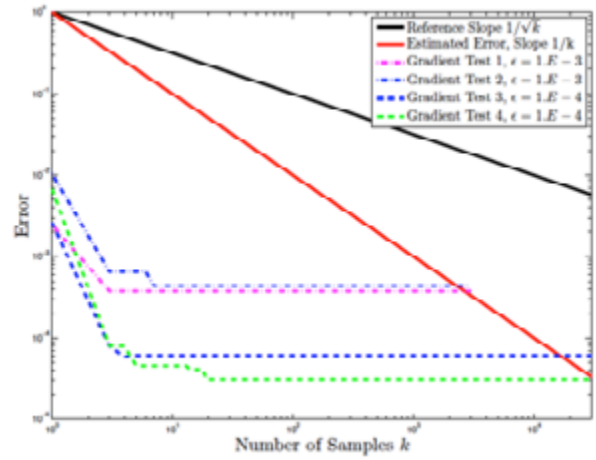


Figure 1: Only a few samples are needed to identify a low dimensional active subspace that preserves the expectation of a QoI to within desired tolerance.

However, in many cases, the response of a quantity of interest (QoI) is dominated by variations of the inputs in a small dimensional active subspace, hence, an efficient procedure that identifies the active subspace would allows us to convert the problem to a low dimensional one and take advantage of the fast SG and qMC methods.

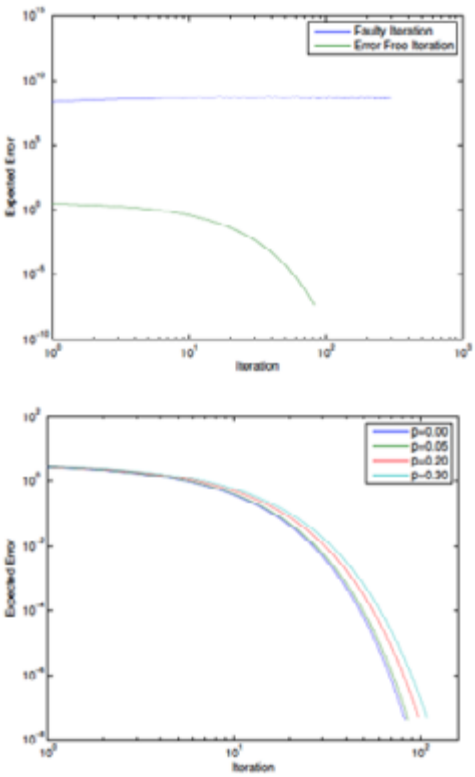
This work was sponsored by Advanced Scientific Computing Research (ASCR): A Mathematical Environment for Quantifying Uncertainty: Integrated and Optimized at the eXtreme scale (EQUINOX), **equinox.ornl.gov**.

Numerical Analysis of Fixed Point Algorithms in the Presence of Hardware Faults

M. Stoyanov and C. Webster

Researchers developed an analytic fault model that allows for accurate prediction of the effects of silent faults on the accuracy of the numerical approximations. They applied their approach to the fixed point iteration and demonstrate that the classical algorithm does not converge in expectation, when executed on unreliable hardware. They preset a modified resilient fixed point method that detects and rejects faults resulting in sharp increase of the numerical error, while faults resulting in small perturbations are negated by the natural self-correcting properties of the contraction. The accept/reject test performed in safe mode has relative low cost, thus, the resilient algorithm can produce reliable results without a significant increase of the computational cost.

This work was supported by Advanced Scientific Computing Research (ASCR): Extreme-scale Algorithms & Solver Resilience (EASIR)



Top: classical Jacobi method executes with and without simulated faults. Bottom: resilient Jacobi method converges even for high fault rate p.

Science Highlights [Continued]

Bound-Preserving Discontinuous Galerkin Methods for Conservative Phase Space Advection

E. Endeve, C.D. Hauck, Y. Xing, (ORNL) and A. Mezzacappa (University of Tennessee)

We have developed a bound-preserving DG method to simulate the advection of neutral particles in phase space using curvilinear coordinates. Proofs that highlight necessary conditions to ensure that the method preserves bounds for the phase space distribution function (i.e., suitable CFL conditions, the use of a high-order limiter, and preservation of a divergence-free property of phase space flow) are presented for general curvilinear coordinates and six dimensions, and the details of these conditions are worked out for some commonly used coordinate systems. Results from numerical experiments demonstrate that the method achieves high-order accuracy and that the physical bounds on the distribution function are satisfied; i.e., $f \in [0, 1]$ (Figure 1).

Discontinuous Galerkin (DG) methods for solving hyperbolic partial differential equations are attractive for several reasons. First, they achieve high-order accuracy on a compact, local stencil so that data is only communicated with nearest neighbors (regardless of the formal order of accuracy), which leads to a high computation to communication ratio. Second, when applied to modeling of transport processes, they recover the correct asymptotic behavior in the diffusion limit — characterized by frequent collisions and long characteristic time scales. To leverage these properties, it is important that the numerical method preserves physical bounds of the underlying model; e.g., positivity of the phase space distribution function f in a kinetic model for non-equilibrium transport. In the case of fermions, f is also bounded above (i.e., $f \leq 1$). Aside from being physically meaningless, violation of these bounds can result in numerical difficulties due to nonlinearities.

Support for this work was provided by Oak Ridge National Laboratory (ORNL) Laboratory Directed Research and Development Program and the National Science Foundation. Computational resources of the Oak Ridge Leadership Computing Facility at ORNL were provided through the INCITE program and a Director's Discretionary allocation.

Read more about this work [**here**]. http://arxiv-web3.library.cornell.edu/abs/1410.7431

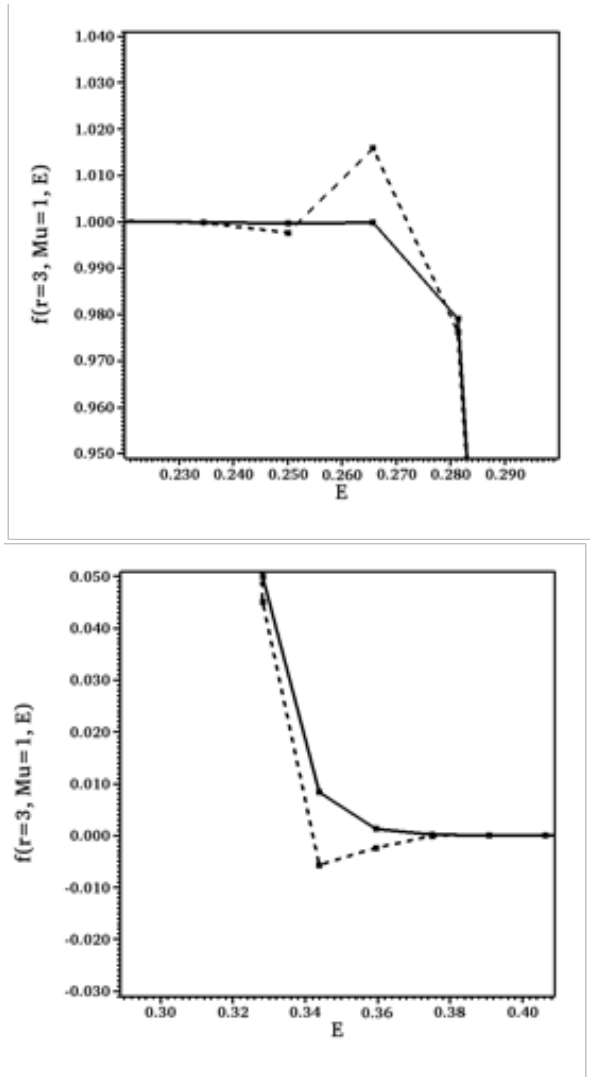


Figure 1: Distribution function f versus energy E for a problem involving a Fermi- Dirac initial distribution (top and bottom).

The distribution function satisfies $f \in [0, 1]$ for all times due to bound-preserving properties of the high-order DG scheme (solid lines). f becomes non-physical oth- erwise (dashed lines).

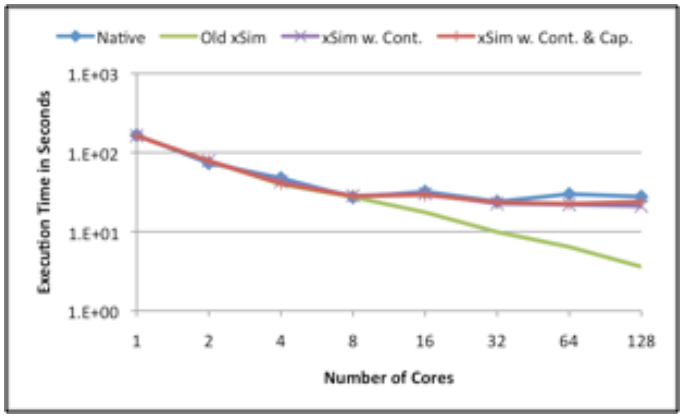
Science Highlights [Continued]

A Network Contention Model for the Extreme-scale Simulator

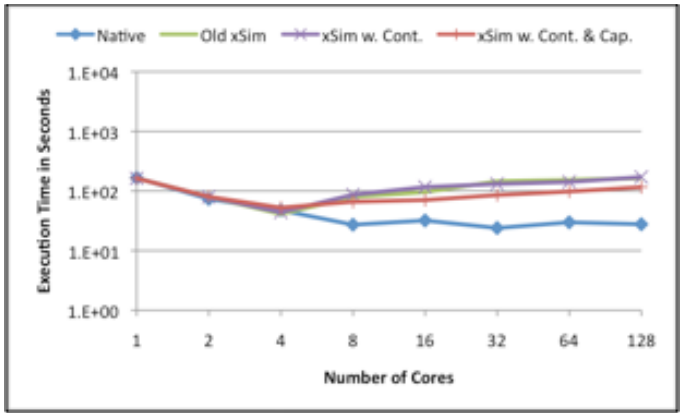
C. Engelmann and T. Naughton

The Extreme-scale Simulator (xSim) is a performance investigation toolkit for high-performance computing (HPC) hardware/software co-design. xSim permits running a HPC application with millions of concurrent execution threads, while observing its performance in a simulated extreme-scale system. This work offers a newly developed network modeling feature for xSim, eliminating the shortcomings of the existing network modeling capabilities. The approach takes a different path for implementing network contention and bandwidth capacity modeling using a less synchronous and accurate enough model design. With the new network modeling feature, xSim is able to simulate on-chip and on-node networks with reasonable accuracy and overheads. The evaluation results of the implemented network contention and bandwidth capacity model show that the simulation error introduced by xSim using the original network model could be reduced from 87% to 26%, for example, for the NAS Parallel Benchmark (NPB) conjugate gradient (CG) solver when simulating a 256-node computer system with 2 processors per node and 4 cores per processor. The additional simulation runtime overheads are minimal, e.g., from 506% to 517% for NPB CG with the network contention model. A reduction of the simulation runtime overhead to 318% can be observed with the additional bandwidth capacity model due to additional internal optimization opportunities in the parallel discrete event simulation.

Work was performed at ORNL and funded by ORNL's Laboratory Directed Research and Development program and DOE's Advanced Scientific Computing Research program.



Native (without xSim in wall-clock time) and simulated NAS Parallel Benchmark (NPB) conjugate gradient (CG) solver performance (in simulated time) with original network model (Old xSim), added network contention model (xSim w. Cont.), and added network bandwidth capacity model (xSim w. Cont. & Cap.)



Native (without xSim in wall-clock time) NPB CG solver and simulator performance (in wall-clock time) with original network model (Old xSim), added network contention model (xSim w. Cont.), and added network bandwidth capacity model (xSim w. Cont. & Cap.)

Science Highlights [Continued]

Conservative Formulations for Simulation of Non-Equilibrium Transport in Dense Nuclear Matter

C.Y. Cardall, E. Endeve, (ORNL) and A. Mezzacappa (University of Tennessee)

We derived conservative forms of the general relativistic Boltzmann equation and associated moment equations in the so-called 3+1 formulation — the most commonly used formulation in numerical relativity. One challenge to overcome when developing numerical methods for neutrino transport to construct a structure- preserving discretization that is faithful to both energy and lepton number conservation (a property that is satisfied analytically by the underlying PDEs). To this end, we have exposed analytical relationships between conservation laws for energy and lepton number in the 3+1 formulation. These developments form the necessary theoretical foundation for development of conservative numerical methods to simulate neutrino transport in systems involving dynamical spacetimes. This work is also relevant to the design of robust, "positivity-preserving" numerical methods (i.e., that preserve positivity of manifestly positive physical quantities).

Conservation laws are ubiquitous in the physical sciences. Mathematically, conservative formulations of physical laws as partial differential equations (PDEs) are convenient when discontinuous solutions can develop. In addition, conservation laws lead naturally to numerical methods with conservation properties. When simulating the transport of neutrinos through dense nuclear matter, e.g., to study element production in core-collapse super- novae or binary neutron star mergers, a kinetic description based on the relativistic Boltzmann equation is needed to capture non-equilibrium effects, since neutrinos interact weakly with matter. To establish confidence in such simulations, it is important to accurately capture the exchange of energy and lepton number between neutrinos and the matter. The total of both quantities must be conserved within tolerance.

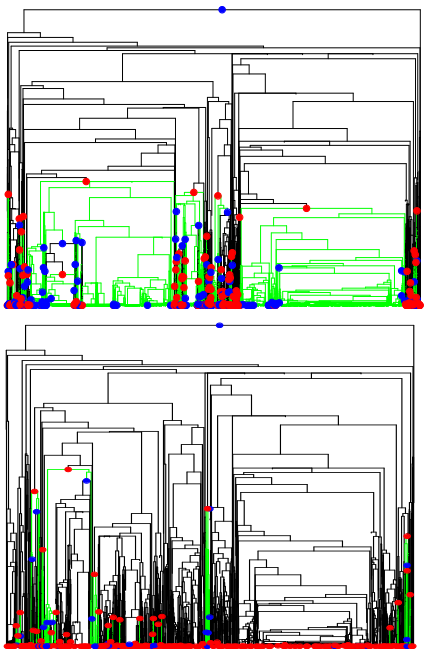
Support for this work was provided by The Office of Advanced Scientific Computing Research and the Office of Nuclear Physics, U.S. Department of Energy.

Read the full document [**here**]. http://journals.aps.org/prd/pdf/10.1103/PhysRevD.87.103004

Protein family database UniFam enables functional phylogenomics analysis, reveals potential pathways in prokaryotic organisms

J. Chai, G. Kora, T.-H. Ahn, D. Hyatt and C. Pan

UniFam is a newly constructed protein family database. Based on UniFam, a new full-length protein annotation pipeline was developed to analyze genomes more consistently and reliably. All the prokaryotic genomes were annotated and their metabolic pathways were inferred. Consistency of each pathway with phylogeny was also assessed.



Subtree for pathways. The root is colored blue for the pathway's absence. The colors of non-root nodes mark the pathway's status changes from their immediate ancestors: red for gains, blue for losses, and none for no change. The branches descending from nodes containing the pathway are colored green. (Top) Pyruvate fermentation to ethanol I. (Bottom) Pyruvate fermentation to ethanol III.

Phylogenomics analysis fully measured the consistency between the evolution of pathways and sequences. It reveals distinct evolutionary patterns for different pathways. Pathways of high inconsistency are potentially capable of undergoing horizontal gene transfer, which can help target organisms and molecular functions of interest.

The functional phylogenomics analysis shows divergent functional profiles of taxa and clades. Such function-phylogeny correlation stems from a set of clade-specific cellular functions with low parsimony scores. On the other hand, many cellular functions are sparsely dispersed across many clades with high parsimony scores. These different types of cellular functions have distinct evolutionary patterns reconstructed from the prokaryotic tree.

For more information, please the publication - J. Chai, G. Kora, T.-H. Ahn, D. Hyatt and C. Pan. "Functional phylogenomics analysis of bacteria and archaea using consistent genome annotation with UniFam", BMC Evolutionary Biology 2014, 14:207.

http://www.biomedcentral.com/1471-2148/14/207

Science Highlights [Continued]

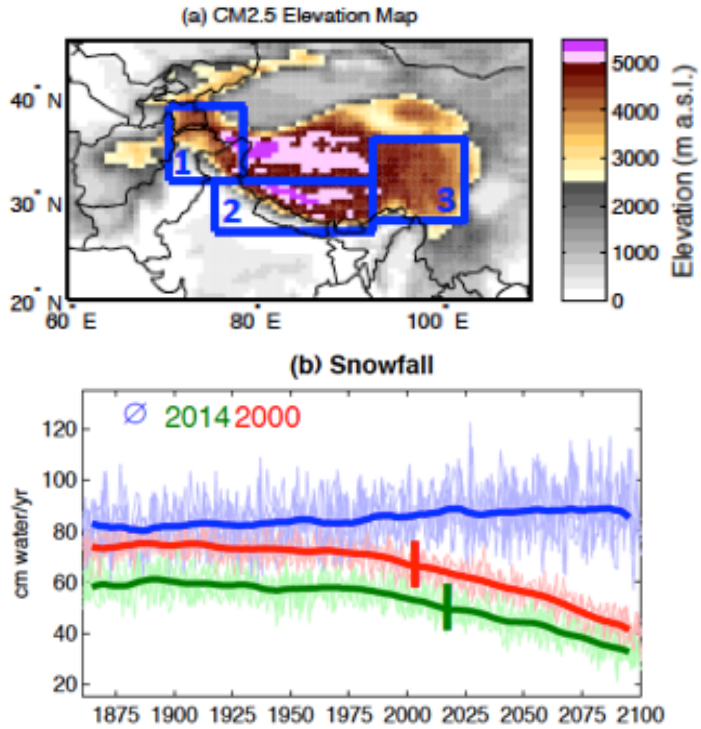
Snowfall Less Sensitive to Warming in Karakoram than in Himalayas Due to a Unique Seasonal Cycle

S. B. Kapnick, T. L. Delworth, M. Ashfaq, S. Malyshev, and P. C. D. Milly

We demonstrated that the Karakoram seasonal cycle is dominated by non-monsoonal winter precipitation, which uniquely protects it from reductions in annual snowfall under climate warming over the twenty-first century. The simulations show that climate change signals are detectable only with long and continuous records, and at specific elevations. Their findings suggest a meteorological mechanism for regional differences in the glacier response to climate warming.

The high mountains of Asia, including the Karakoram, Himalayas and Tibetan Plateau, combine to form a region of perplexing hydroclimate changes. Glaciers have exhibited mass stability or even expansion in the Karakoram region1–3, contrasting with glacial mass loss across the nearby Himalayas and Tibetan Plateau1,4, a pattern that has been termed the Karakoram anomaly. However, the remote location, complex terrain and multi-country fabric of high-mountain Asia have made it difficult to maintain longer-term monitoring systems of the meteorological components that may have influenced glacial change. Here the researchers compare a set of high-resolution climate model simulations from 1861 to 2100 with the latest available observations to focus on the distinct seasonal cycles and resulting climate change signatures of Asia's high-mountain ranges.

This work was performed at the Geophysical Fluid Dynamics Laboratory, ORNL, and USGS



Elevation map (top) region 1 represents the region with Karakoram anomaly. Snowfall trend (bottom) from 1860 to 2100 over three regions. Blue color represents the Karakoram region and vertical lines represent the year when the trend is significant. Karakoram region doesn't show any significant trend through the 21st century.

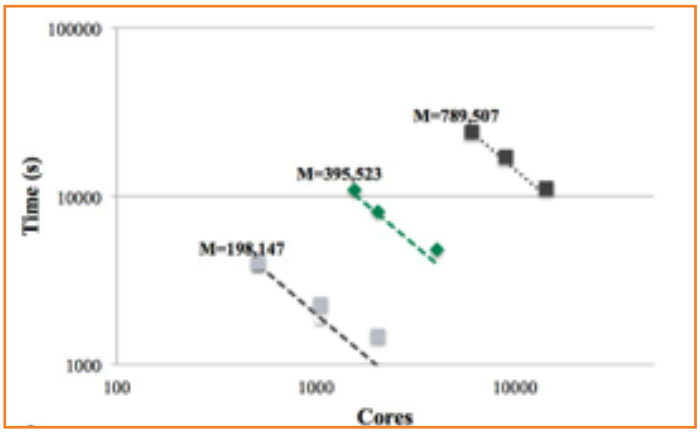
Read more about this work [**here**]. http://www.nature.com/ngeo/journal/v7/n11/full/ngeo2269.html

Parallel Out-of-Core Dense Matrix Factorization on GPU and Intel MIC

E. D'Azevedo and Judy Hill

Researchers have developed a parallel out-of-core LU and Cholesky factorization algorithm that can be used as a replacement for ScaLAPACK solvers. The solver has been ported to run on Nvidia K20 GPU on the Cray XK7 Titan supercomputer and for Intel MIC on the Beacon cluster at the National Institute for Computational Sciences (NICS) at the University of Tennessee. The algorithm can also be adapted to be used as a benchmark to evaluate different approaches for programming the accelerators such as OpenMP target directives, Intel offload directives, OpenACC directives, and Nvidia Compute Unified Device Architecture (CUDA).

This work is supported by Laboratory Directed Research and Development: MiniApps: Building Laboratories for Portable Performance from the Petascale to the Exascale.

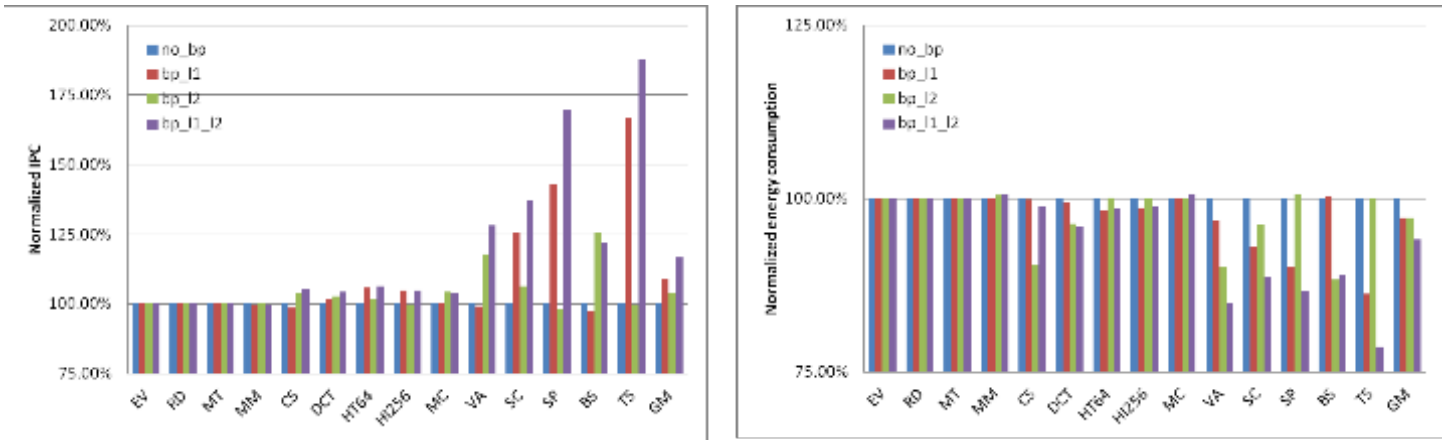


Performance of AORSA using parallel out-of-core solver using GPU acceleration on Cray XK7 Titan

Science Highlights [Continued]

RACB: Resource Aware Cache Bypass on GPUs

Hongwen Dai (North Carolina State University), Christos Kartsaklis, Chao Li (North Carolina State University), Tomislav Janjusic, Huiyang Zhou (North Carlolina State University)



The impact on performance (left) and the total energy savings (right) from resource-aware cache bypass (RACB) for a suite of 14benchmark applications. Performance is measured as the number of instructions per cycle, relative to the non-RACB case (higher is better). Energy is measured relative to the non-RACB case (lower is better). In both graphs, individual bars represent different bypass scenarios (none, L1-data cache only, L2 cache only, and both L1 and L2 together).

In this work, the researchers developed a mechanism, termed Resource Aware Cache Bypass (RACB), that would allow a GPU to automatically detect when memory cache is hindering its performance and switch to a mode that bypasses the cache in order to allow processing to continue. When the problem passes, the GPU returns to using the cache, as usual. Because this is a change to the system hardware, the researchers evaluated it using a popular GPU simulation package, GPGPUSim, configured to model an NVIDIA GTX480 processor. The evaluation involved fourteen different benchmark applications which are part of the NVIDIA CUDA SDK, and which represent a number of common motifs in scientific and technical computing. They compared the performance of the base system (no bypass capability) to using the proposed RACB mechanism for either the L1-data cache only, the L2 cache only, or both caches together. The results indicate that RACB for both caches together provides the most benefit, both for performance (16.7% improvement on average, 88.0% best case), and energy consumption (5.9% average, 22.4% best), while having a negligible impact on normal operation of the GPU.

This work was performed at ORNL, OLCF, and North Carolina State University.

For more information, please go [**here**].

http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=6972010

Science Highlights [Continued]

Nonlinear Collision Becomes Practical from Multi-Threading

Ed D'Azevedo (ORNL) and Patrick Worley (ORNL)

Researchers, through the effective use of OpenMP on multiple CPU cores, were able to accelerate the Fokker-Planck collision module by nearly five times while reducing the overall time in XGC1 by 1.7 times. This new accelerated collision module enables higher fidelity prediction for ITER's fusion performance by account for non-equilibrium edge plasma.

Working with Patrick Worley in the SciDAC Institute for Sustained Performance (SUPER) to perform performance profiling to find opportunities for optimization, the team identified there is load imbalance and insufficient work per grid cell to fully exploit OpenMP parallelism. The Fokker-Planck collision module is restructured to use OpenMP processing across multiple computational grid cells. Moreover, the team collaborated with Barry Smith, developer of PETSc (Portable, Extensible Toolkit for Scientific Computing) in the SciDAC FastMath Institute, to obtain a special thread-safe version of PETSc. Another thread-safe solver based on LAPACK band solver was also developed. The National Transport Code Collaboration (NTCC) pspline cublic spline library was also modified to be thread-safe.

The XGC1 is a first-principles kinetic particle-in-cell (PIC) code developed in the Center for Edge Physics Simulation (EPSI) project in the Department of Energy Scientific Discovery through Advanced Computing (SciDAC) program. The application is used for understanding the turbulent plasma transport near the edge region of a tokomak fusion device. The success of ITER (International Thermonuclear Experimental Reactor) is critically dependent upon effective confinement of high temperature plasma, especially near the edge region.

	Main loop time	Collision routine time
Multi threaded collision	200 s	32 s
Single threaded collision	340 s	171 s

Summary of time for 10 time steps in XGC1 on Cray XK7 Titan.

As the physics models are refined and enhanced, the performance kernels of the XGC code will evolve as well. The activation of a new Fokker-Planck-Landau collision physics on highly non-Maxwellian edge plasma nearly doubled the overall computation time.

This work was sponsored by:

- Advanced Scientific Computing Research (ASCR) SciDAC and Fusion Energy Sciences (FES): Center for Edge Physics Simulation (EPSI) **epsi.pppl.gov**
- Advanced Scientific Computing Research (ASCR): SciDAC Institute for Sustained Performance, Energy, and Resilience (SUPER) **www.super-scidac.org**
- Office of Science Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program
- http://www.doeleadershipcomputing.org/incite-program/

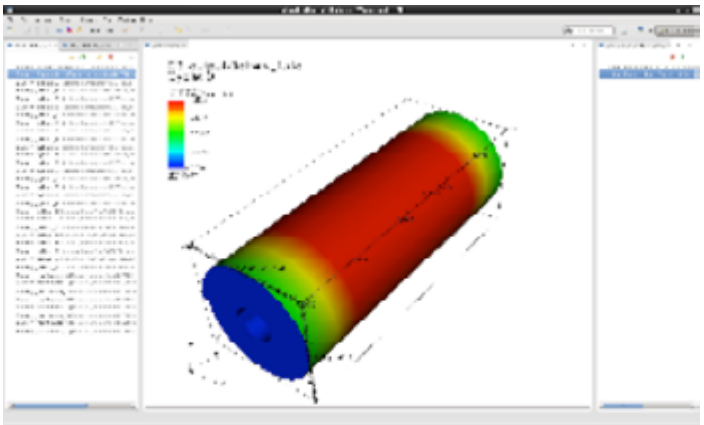
Advanced 2D and 3D Visualizations in Eclipse ICE with VisIt and JavaFX

Taylor Patterson, Jordan H. Deyton, Harinarayan Krishnan, Alexander J. McCaskey, Anna Wojtowicz, and Jay Jay Billings

Researchers developed tools within the Eclipse Integrated Computational Environment (ICE) to allow users to generate 2D and 3D graphical views rendered by the VisIt visualization tool and JavaFX 8. This work enhances the capabilities of ICE to provide robust, 2D and 3D scientific visualization software to users for data analysis within the same, standardized application where they prepare simulation input and execute the simulation run.

This work was performed at ORNL and LBNL under the sponsorship of the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program.

View the presentation materials [here]. https://www.eclipsecon.org/europe2014/sites/default/files/slides/patterson_ECESlides.pdf



This temperature profile of a cylindrical battery cell is rendered by VisIt and displayed in ICE.

Science Highlights [Continued]

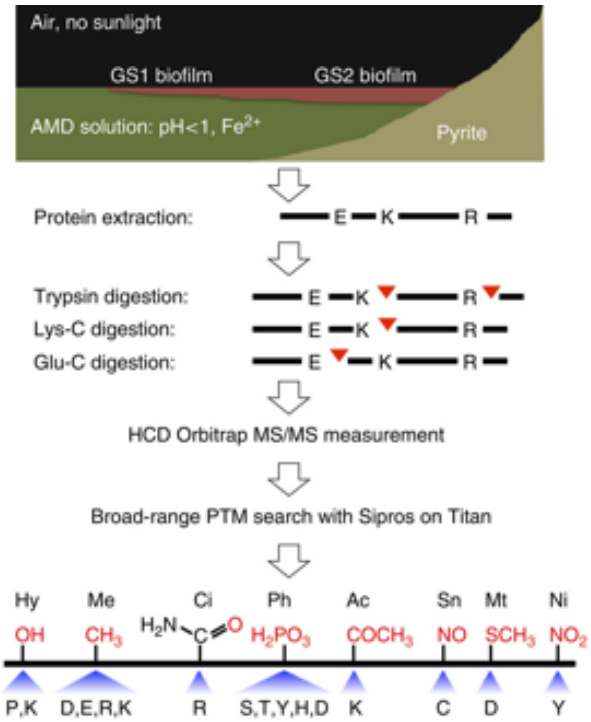
Role of Post-Translational Protein Modification in Community-Scale Processes

Zhou Li, Yingfeng Wang, Qiuming Yao, Nicholas B. Justice, Tae-Hyuk Ahn, Dong Xu, Robert L. Hettich, Jillian F. Banfield and Chongle Pan

In this study, a collaborative team of researchers at the Oak Ridge National Laboratory, University of Tennessee-Knoxville, University of California-Berkley and University of Missouri-Columbia developed a novel technique that allows PTM analysis in proteins collected from an intact microbial community (i.e., the metaproteome) using high-resolution mass spectrometry coupled to high-performance computing. The investigators examined PTM in a model biofilm community found in a highly acidic environment and were able to link this regulatory mechanism to several community-scale phenotypes that could not be explained by observed changes in gene expression. Community-level attributes associated with PTM in this study included alterations in community structure, nutrient acquisition strategies, and resistance to viral invasion. This finding represents a considerable advance in the application of systems biology approaches to community-level analysis. The team now is working to scale up this technique to enable investigations of more complex communities and environments.

This work was funded by the US Department of Energy Office of Science, Biological and Environmental Research, Carbon Cycling program and Knowledgebase program and National Institutes of Health grant. The database searching for identification of protein post-translational modifications was performed on the Oak Ridge Leadership Computing Facility-Titan.

For more information, please click [**here**]. http://www.nature.com/ncomms/2014/140725/ncomms5405/full/ncomms5405.html



AMD biofilms representing two growth stages (GS1 and GS2) were collected from a site within the Richmond Mind. Proteome samples were digested using three proteases in parallel and analysed by HCD MS/MS. The following biological PTMs were searched: hydroxylation (Hy), methylation (Me), citrullination (Ci), phosphorylation (Ph), acetylation (Ac), S-nitrosylation (Sn), methylthiolation (Mt) and nitration (Ni). The chemical formula (red) and modifiable amino acids are listed for each type of PTM.

Science Highlights [Continued]

Dynamic Charge Storage in Ionic Liquids-filled Nanopores: Insights from a Computational Cyclic Voltammetry Study

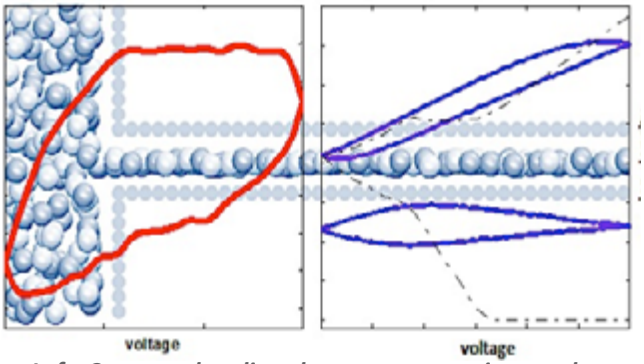
Yadong He, Jingsong Huang, Bobby G. Sumpter, Alexei A. Kornyshev, and Rui Qiao

Computer simulations allowed probing directly dynamic charge storage at the single-pore level both spatially and temporally, which is extremely difficult, if possible at all, to access experimentally.

The understanding of the mechanisms underlying the dynamical phenomena and their effects on the energy density and efficiency of the dynamic charge storage in nanopores provides a means to improve supercapacitor performance.

This work was performed at the Center for Nanophase Materials Sciences, Virginia Tech, and Imperial College London.

Read the full document [**here**]. http://pubs.acs.org/doi/abs/10.1021/jz5024306



Left: Computed cyclic voltammetry superimposed on representative snapshots taken from molecular dynamics simulations for the charging/discharging of a carbon nanopore with a RTIL. Right: Evolution of the average counterion and co-ion densities inside the pore during the steady-state charging/discharging cycles.

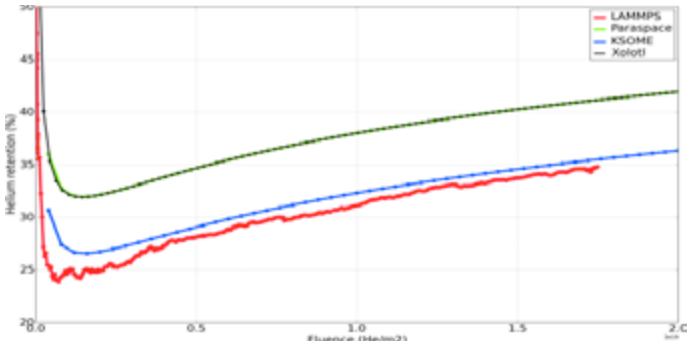
Xolotl Plasma-Surface Simulator Code Cross-Comparison

S. Blondel, A. Belt, D. Bernholdt, J. Billings, K. Hammond, D. Higdon, C. Jernigan, O. Knio, A. McCaskey, J. Meredith, H. Najm, P. Roth, K. Sargsyan, B. Smith, B. Wirth, D. Xu, T. Yamaguchi-Phillips, Z. Yang

The Plasma-Surface Interactions SciDAC project is focused on predicting material damage in plasma-facing components in tokamak fusion reactors. Xolotol is a new continuum advection-reaction-diffusion cluster dynamics simulation code, which is intended extend modeling capabilities to the time and spatial scales relevant for systems such as the tungsten plasma divertor planned for the ITER tokamak.

Because the experimental environment, even in simplified, lower-energy, "linear" plasma devices is quite complex, we are carrying out detailed cross-comparisons to other simulation codes as an important component of the process of verification and validation of Xolotl. Three applications have been selected for these cross-comparisons. Paraspace is an independent implementation of the same continuum reaction-diffusion model initially implemented in Xolotl. KSOME uses a kinetic Monte Carlo (KMC) approach to model the system, but utilizes a very similar reaction network to model the system. And finally, the LAMMPS molecular dynamics (MD) package provides much more detailed atomistic modeling of the system.

The figure above is representative of the results observed in our initial cross-comparison. Xolotl and Paraspace give essentially identical results, as expected. The KMC and MD results show the general same trends as Xolotl, but



This figure shows the helium retention percentage (quantity of helium retained in the tungsten material divided by the fluence of helium) as a function of the helium fluence, for the four different simulation codes with the same running conditions: tungsten (001) oriented material of 25nm thick irradiated by a helium flux of 4.0 x 1025 He/m2/s. The results from Paraspace and Xolotl coincide.

are different in detail. Such differences are expected, since Xolotl does not yet include all of the physics included in the KMC and MD models. Advection processes have recently been added to Xolotol, and work is underway on bubble bursting, cluster coalescence, loop punching, and surface growth. Additional comparisons with MD and KMC results as these features are added to Xolotl will assist with their verification.

This work was performed at ORNL and UTK as part of the SciDAC Plasma-Surface Interactions project, jointly sponsored by Fusion Energy Sciences (FES) and Advanced Scientific Computing Research (ASCR) programs within the U.S. Department of Energy Office of Science.

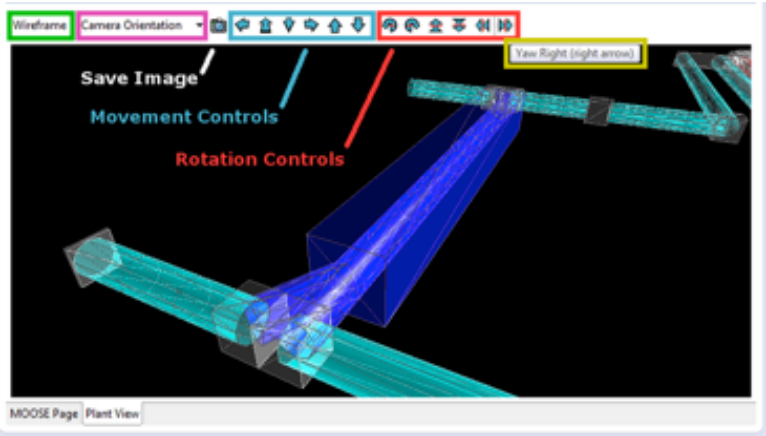
Science Highlights [Continued]

Eclipse ICE Improves Support for MOOSE-Based RELAP-7

Alex McCaskey, Anna Wojtowicz, Jordan H. Deyton, Taylor Patterson, Jay Jay Billings

The Eclipse Integrated Computational Environment (ICE) team has spent the first quarter of FY15 drastically improving support for the RELAP-7 MOOSE application. RELAP-7 represents an update to the venerable RELAP-5 simulator that is built upon the MOOSE framework and attempts to model the balance-of-plant concerns in a full nuclear plant. The development effort focused on improvements, bug fixes, and feature additions to existing MOOSE-based application support and RELAP-7 specific capabilities. Considerable work was done to improve the MOOSE Model Builder, the MOOSE Job Launcher, and the 3D Nuclear Plant Viewer (see screenshot). The team also developed a brand new Eclipse Perspective for MOOSE users that clears away un-related buttons and widgets so that MOOSE users can get directly to the data they care about.

The MOOSE Model Builder now includes support for discrete parameter editing and functionality for automatically generating the metadata necessary to describe a RELAP-7 input file (this was previously left as a task for the user). It also contains a dynamic and interactive 3D Plant Viewer that was updated with support for saving plant images, changing the camera orientation and position, and wireframe toggling.



RELAP-7 users will also find improved post-simulation data visualization support with enhancements to the ICE VisIt visualization functionality, specifically the ability to view different types of VisIt plots (mesh, pseudocolor, contour, etc.). Additionally, users can now take MOOSE PostProcessor CSV data from a simulation and plot it natively within ICE through the ICE CSV Plotting tool.

This work was performed at ORNL under the sponsorship of the Department of Energy Office of Nuclear Energy Nuclear Energy Advanced Modeling and Simulation (NEAMS) program.

Image Reconstruction from Fourier Data Using Sparsity of Edges

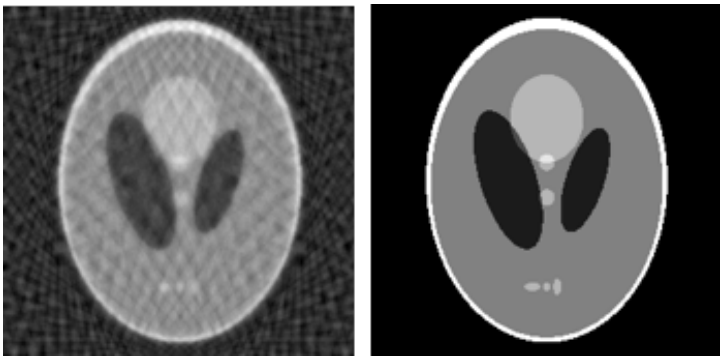
Richard Archibald

We use the polynomial annihilation edge detection method to generate the corresponding sparsifying transform. Our method successfully reduces the Gibbs phenomenon with only minimal blurring at the discontinuities while retaining a high rate of convergence in smooth regions.

This work lays the foundations for high order sparse reconstruction of piecewise smooth images from Fourier samples, such is the case for neutron tomography. Advancing the mathematics of neutron tomography will provide freedom to design fast scanning methods that will allow novel scanning methods that can sparsely sample in reciprocal space while maintaining image fidelity.

This work was sponsored by Advanced Scientific Computing Research (ASCR): ACcurate qUantified Mathematical mEthods for Neutron science (ACUMEN).

Read the full document [**here**]. http://link.springer.com/article/10.1007%2Fs10915-014-9973-3



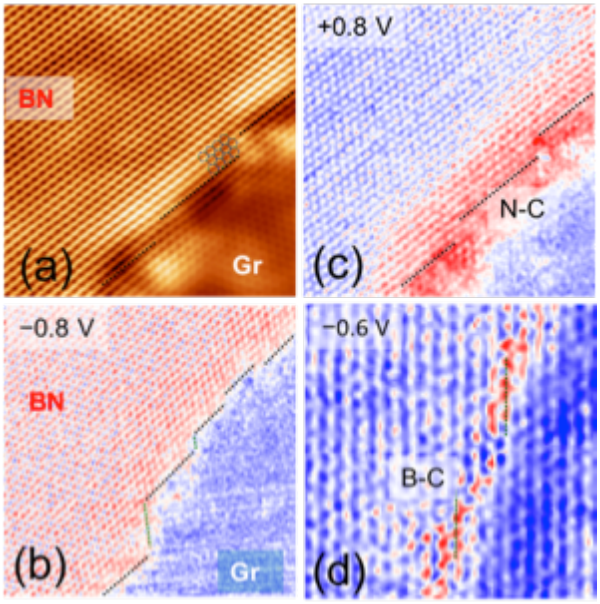
Left: Standard filtered back projection reconstruction. Right: Sparse Optimization of Shepp Logan Phantom

Science Highlights [Continued]

Spatially Resolved One-Dimensional Boundary States in Graphene-Hexagonal Boron Nitride Planar Heterostructures

Jewook Park, Jaekwang Lee, Lei Liu, Kendal W. Clark, Corentin Durand, Changwon Park, Bobby G. Sumpter, Arthur P. Baddorf, Ali Mohsin, Mina Yoon, Gong Gu, and An-Ping Li

The extensive research on the two-dimensional (2D) interface between different materials, such as complex oxides, has led to the discovery of a number of new physical phenomena not seen in the constituent 3D crystals. The advent of graphene and other 2D crystals brings about the expectation that similarly interesting physics may arise at the 1D interface between 2D crystals. The teams work provides the first glimpse into 1D boundary states formed by two prototypical 2D materials: single-layer graphene and hexagonal boron nitride (hBN). From atomic resolution scanning tunneling microscopy (STM) images and spectroscopy (STS), they found that the boundary states are about 0.6 eV away from the Fermi level, extended along and localized at the boundary with a spatial width of a few atomic lattices. Both the spatial and energetic distributions of the 1D boundary states are strongly associated with boundary terminations, orbital mixing, asymmetric screening, and the polarity-induced electric field. This work allows the team to discuss the implication of the "polar catastrophe" at a 1D interface for the first time, and opens a route for new low-dimensional physics and tuning of electronic properties at interfaces in 2D heterostructures.



(a) STM image showing atomic structure of in-plane graphene-hexagonal BN monolayer junction. (b) Atomically resolved electronic density of states. (c) Boundary states (red color) at the interface terminated primarily by nitrogen. (d) Boundary states at the interface terminated primarily by boron.

This work was performed at the Center for Nanophase Materials Sciences and the University of Tennessee.

For more information, please click [**here**]. http://www.nature.com/ncomms/2014/141107/ncomms6403/abs/ncomms6403.html

Science Highlights [Continued]

Generalized methodology for analyzing quasi-optimal polynomial approximations for parameterized PDEs with deterministic and stochastic coefficients

R. DeVore, H. Tran, C. Webster, and G. Zhang

The team demonstrated a novel, generalized methodology that is applicable to analyze most of published quasi-optimal approximations. Compared to previous approaches, their framework was shown to be advantageous in that: i) it gave sharp estimates of the asymptotic convergence rates (see Figure 1) and, ii) it applied to many quasi-optimal methods that cannot be treated by current error analyses.

In their paper, Analysis of Quasi-optimal Polynomial Approximations for Parameterized PDEs with Deterministic and Stochastic Coefficients, the research team investigates simultaneously solving the entire family of parameterized partial differential equations by global-based polynomial approximations. For such methods, an effective construction of polynomial subspaces, which yields maximum accuracy for a given computational cost, is desirable. The goal of selecting the best subspaces and index sets is, however, not feasible in high dimensional problems, since it requires the computation of all of the polynomial coefficients. Quasi-optimal approximations, choosing the index sets that corresponds to the "best M-terms" based on sharp estimates instead of exact calculations of the coefficients, is an attractive alternative to alleviate the high cost of the optimal method.

Under some weak assumptions on the coefficient bound (which are satisfied by all existing coefficient estimates we are aware of), the team achieve an asymptotic sub-

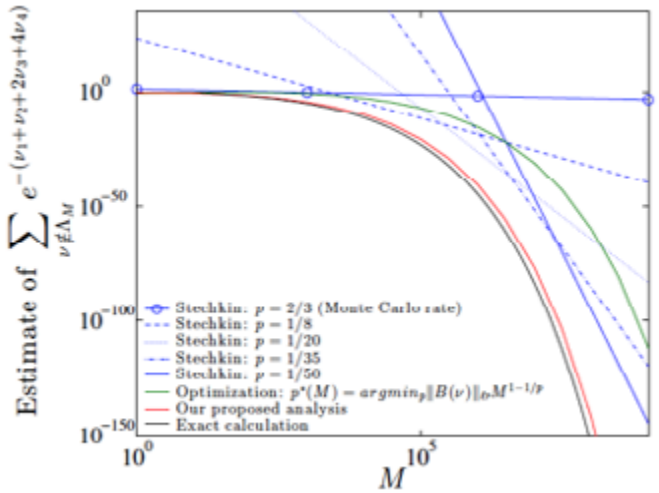


Figure 1: A comparison of our error estimate with those resulting from previous approaches

exponential convergence rate of truncation error of the form M exp(−(κM)1/N), where κ is a constant depending on the shape and size of quasi-optimal index sets. Through several examples, they explicitly derive κ and demonstrate the optimality of their estimate both theoretically (by proving a lower bound) and computationally (via comparison with exact calculation of truncation error).

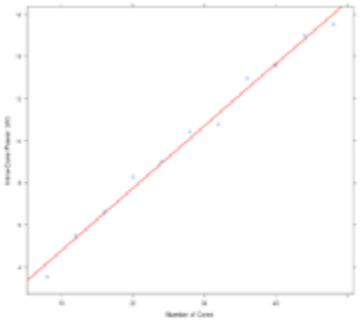
Support for this paper was provided by the Air Force Office of Scientific Research (AFOSR): Advanced uncertainty quantification methods for predictive simulations of stochastic turbulence systems.

Data Motion Power Model

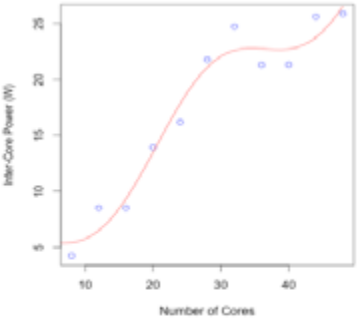
Tiffany M. Mintz, Stephen W. Poole, and Tosin O. Alabi

Researchers derived functions that serve as a preliminary model for core level data motion power costs. In this first year of research, the researchers focused on data motion at the core level. The core level model will provide the basis for node and cluster level modeling of data motion power consumption. The primary task this year was data collection. In order to collect data, they had to select an appropriate tool for measuring component level power consumption in multicore architectures. The researchers decided that simulation tools would provide the necessary flexibility for gathering component level power data across various multicore architectures. To this end, they completed an extensive survey of simulation frameworks with power measurement capabilities.

Of the many simulators surveyed, preliminary experiments were performed on SST, Graphite and Sniper. The sniper simulator proved to be the most suitable framework for component-level, multicore power measurements. The researchers performed a comprehensive set of experiments using multiple applications over a range of core counts and varying memory protocols. These experiments generated sufficiently large and diverse data sets for deriving the desired cost model, which has been added to the ESSC



An Intra-core linear power model derived from the power data: Intra_Power = 0.295695*Num_ Cores + 1.820636



An Intra-core linear-sine power model derived from the power data: Inter_Power = 3.037384 + 0.5392907*Num_Cores + 2.9968409 * sin(2 * 3.141593 * (Num_Cores – 24.1292520)/-0.3299030)

Database. Linear, inverse and linear-sine regression analysis has been performed on the power data, with functions derived to model the multicore data motion power consumption.

This work was sponsored by the Department of Defense.

Software

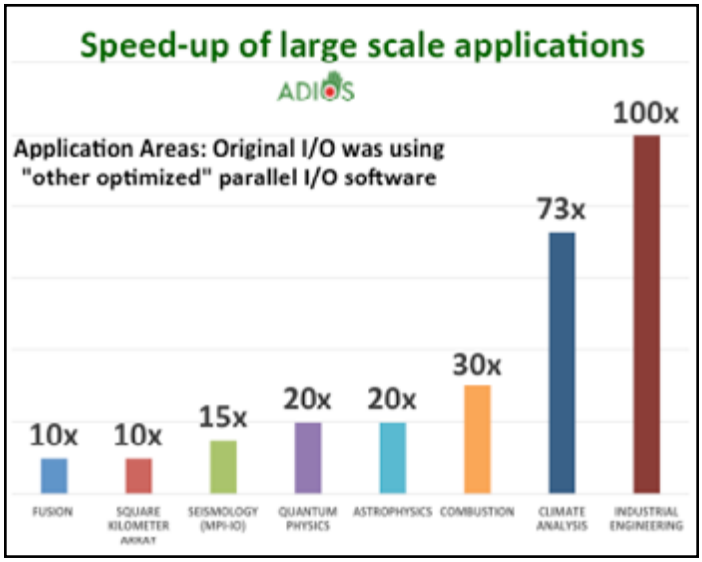
Adios 1.8 Released

S. Klasky, N. Podhorszki, Q. Liu, H. Abbasi, J. Choi, Y. Tian, J. Mu, J. Logan, D. Pugmire, G. Ostrouchov, T. Kurc, I. Rodero, M. Ainsworth, K. Wu, J. Gu, N. Samatova, D. Boyuka, X. Zu, H. Tang, K. Schwan, M. Wolf, G. Eisenhauer, J. Dayal, M. Parashar, H. Bui, F. Zhang, T. Jin, Q. Sun

The Adaptable IO System (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.

Version 1.8 introduces a Query API, which extends the reading capability by formulating a query and by reducing the size of the data that needs to be retrieved from storage. The query interface was developed by ORNL, LBNL and NCSU. A wide-area-network data movement I/O method was developed and added to ADIOS 1.8 by ORNL, Georgia Tech and Rutgers University. Further, a timing profile and timing event recording was added to ADIOS 1.8 that is saved with the output data automatically. It allows analyzing the behavior of the I/O.

Please go [**here**] (https://www.olcf.ornl.gov/center-projects/adios/) for more information.



ADIOS has improved the I/O performance of many large scale applications

VIBE production version 1.0 of ORNL EV battery simulation software released

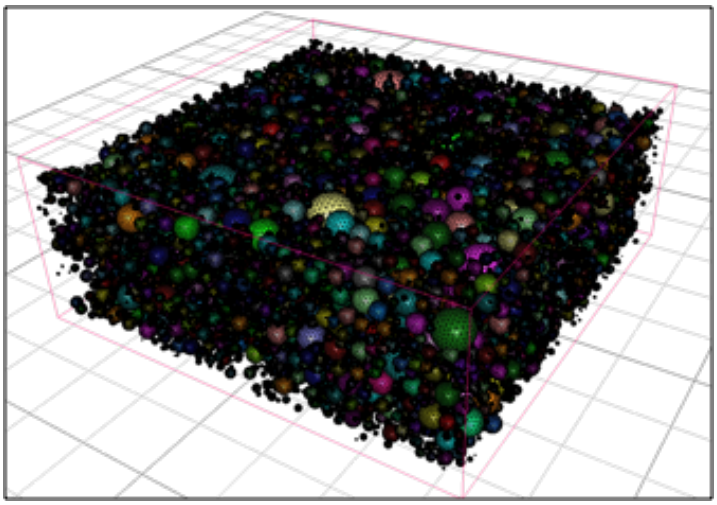
S. Kalnaus, S. Pannala, S. Allu, W. Elwasif, S. Simunovic, J.J. Billings, and J. Turner

Oak Ridge National Laboratory's (ORNL's) Computer-Aided Engineering for Batteries (CAEBAT) team has released a new computational toolset for academic, national laboratory, and industry users to accelerate the design of high-performing, safe batteries for electric vehicles.

The software can accurately simulate key battery performance indicators including charge and thermal transport, electrochemical reactions, and mechanical stresses on the cell sandwich level up to cells, modules, and packs.

"We developed integrated tools so that one doesn't have to employ different performance models for different applications," said Sreekanth Pannala, distinguished research staff member at ORNL. "A materials' developer might need a cell sandwich simulation; a cell manufacturer might only be looking at the cell or a module; whereas an original equipment manufacturer who is interested in the complete battery might look at modules and packs."

Users can run CAEBAT on multiple platforms, from workstations to computing clusters, depending on the complexity of the problem.



Micro-mechanics simulations of the electrode particles

CAEBAT is available for download on a new public website. Researchers at ORNL will provide support to users and improve the software based on community feedback. The CAEBAT project is funded by the DOE Vehicle Technologies Office.

New Projects

LDRD: National Extreme Events Data and Research Center (NEED)-Transforming the national capability for resilience to extreme weather and climate events.

PI: Dale Kaiser, ESD (Kate Evans and Jiang co-I's in CSMD)

The ORNL Climate Change Science Institute (CCSI) will develop and implement a novel concept to transform how the United States studies and prepares for extreme weather events in the context of a changing climate the National Extreme Events Data and Research Center (NEED). The goal of this project is to position ORNL-NEED as the home within both DOE and the federal government for integrated research and tool development for resiliency to climate- and weather-related extreme events, while supporting novel approaches to basic and applied research on forecasting of and adaptation to such events. The project will integrate two distinct components (1) A new "knowledge-base" compiling global historical data on weather- and climate-related extreme events along with a synthesis of knowledge regarding corresponding impacts, costs, and recovery information, as well as scientific research on each event (2). A novel extreme weather events analysis and forecasting approach that will leverage the NEED knowledge-base. This approach is called "Monster Ridges" (MR) in reference to the strong upper-atmosphere ridging patterns typically associated with many types of extreme events. Our preliminary analyses indicate that these ridging patterns have changed over the past three decades in ways that suggest more extreme events.

DOE BER: Large-Scale Organization and Scale-Interaction: A Dynamical Pathway toward Understanding, Modeling and Predicting Energy and Water Cycle Extremes

Site PI: Kate Evans

Extreme weather events (EWE) related to variations in the energy and water cycles have important societal consequences for US residents. EWEs include extreme temperature events such as cold air outbreaks and heat waves as well as extreme precipitation events such as floods and droughts. The frequency of EWEs is strongly impacted by planetary-scale climate modes such as El-Nino Southern Oscillation or the Pacific Decadal Oscillation. They are insufficient, however, in producing EWEs by themselves and intermediary large-scale meteorological patterns such as atmospheric blocking events, cyclones, and polar anticyclones are required for their occurrence. The proposed research is a collaborative effort between Georgia Tech and DOE's ORNL aimed at addressing the above knowledge shortcomings in relation to DOE RGCM research priorities. The research will focus on the following energy and water cycle extremes: winter cold air outbreaks and warm waves, summer heat waves, and droughts and floods. The initial stages of our research will employ atmospheric observational data and concentrate on (a) objectively characterizing LMPs associated with different classes of EWEs and (b) developing simple and concise atmospheric circulation metrics. The second part of our project consists of a detailed diagnosis of the physical mechanisms by which large scale patterns form, produce EWEs and are modulated through the natural modes of climate variability. Inferences will be based on the collective consideration of a suite of dynamical diagnostic tools geared to assess the sources for large-scale atmospheric Circulation patterns occurring in extratropical latitudes. The third part of our project is the parallel study of EWEs in historical and future CGCM simulations. The emphasis will be on studies of CMIP5 simulations and DOE model development efforts related to CESM. There is particular interest in the emerging high resolution (1/4° atmosphere; 1/10° ocean) coupled model simulations to study the benefits gained through model resolution increase. The results will provide valuable information for model improvement. The last portion of our study will be focused on isolating future changes in EWE behavior and the evolving role(s) of larger scale features in enacting these changes.

News

MODELING – Glacial mystery no more …

Moet Ashfaq

By analyzing a computer model output with four times the resolution of previous models, a team of researchers has perhaps explained what has been considered a serious inconsistency in the 2007 Intergovernmental Panel on Climate Change report. The findings, reported by a team that includes scientists from Oak Ridge National Laboratory and Princeton University, explain why glaciers in the Karakoram Range of the Himalayas have remained stable while nearby glaciers have been receding. By examining the region in 50-kilometer pieces instead of 210-kilometer squares, researchers were better able to take into account the Karakoram Range's distinct peaks and valleys. This combined with the Karakoram season cycle dominated by non-monsoonal winter precipitation protects it from reductions in annual snowfall under climate warming. "Our findings suggest a meteorological mechanism for regional differences in the glacier response to climate warming," said ORNL's Moet Ashfaq. The study, which appears in Nature Geoscience, could explain why the Himalayan glaciers aren't likely to succumb to climate change by 2035 as had been predicted by the IPCC. [Contact: Ron Walli, (865) 576-0226; wallira@ornl.gov]

Computational tool lowers cost, improves exploration accuracy

Clayton Webster

A new computational tool developed at Oak Ridge National Laboratory can take some of the cost and guesswork out of oil and gas exploration.

Clayton Webster, Oak Ridge senior scientist and leader of

News [Continued]

the computational and applied mathematics group, said the new approach uses a multilevel Monte Carlo method involving computational algorithms. Repeated random sampling with the tool provides a more accurate picture of the earth's subsurface.

"What we wanted to do is reduce the overall uncertainty or the confidence in where drills are placed and where we get the biggest bang for our buck," Webster said.

According to Webster, the computational tool developed by the Oak Ridge research team is a perfect fit for oil and gas exploration.

Read the entire article [**here**]. http://www.thebakken.com/articles/896/computational-tool-lowers-cost-improves-exploration-accuracy

Events

PAST

CSMD Seminars

http://www.csm.ornl.gov/newsite/events.html#seminars

- December 19, 2014 - Soumi Manna: Evaluating the Performance of the Community Atmosphere Model at High Resolutions
- December 12, 2014 - Jay Jay Billings: Eclipse ICE: ORNL's Modeling and Simulation User Environment
- December 12, 2014 - Andrew Ross: Large scale Foundation Nurtured Collaboration
- December 10, 2014 - Beth Plale: The Research Data Alliance: Progress and Promise in Global Data Sharing
- November 14, 2014 - Taisuke Boku: Tightly Coupled Accelerators: A very low latency communication system on GPU cluster and parallel programming
- November 13, 2014 - Eric Lingerfelt: Accelerating Scientific Discovery with the Bellerophon Software System
- November 12, 2014 - John Springer: Discovery Advancements Through Data Analytics
- November 10, 2014 - Christopher Rodrigues: High-Level Accelerator-Style Programming of Clusters with Triolet
- November 3, 2014 - Benjamin Lee: Statistical Methods for Hardware-Software Co-Design
- October 28, 2014 - Robinson Pino: New Program Directions for Advanced Scientific Computing Research (ASCR)
- October 24, 2014 - Qingang Xiong: Computational Fluid Dynamics Simulation of Biomass Fast Pyrolysis - From Particle Scale to Reactor Scale
- October 23, 2014 - Liang Zhou: Multivariate Transfer Function Design
- October 20, 2014 - John Schmisseur: New HORIzONS: A Vision for Future Aerospace Capabilities within the University of Tennessee
- October 14, 2014 - Krishna Chaitanya Gurijala: Shaped-Based Analysis

The OpenSHMEM User Group (OUG 2014) (Held in conjunction with PGAS 2014, October 7, 2014, Eugene, OR, USA)

Steve Poole, Manjunath Gorentla Venkata, Oscar Hernandez, and Pavel Shamis

This was the first workshop dedicated for the discussion and development of OpenSHMEM specification. The workshop had participation from DoD, DoE Office of Science, National Laboratories, Universities, and computer vendors. The workshop accepted ten work-in-progress papers, and the accepted papers are published as SIGHPC proceedings. The top-rated papers will be invited for a special issue of Scientific Programming journal.

The meeting included ten paper presentations and two invited industry talks from Mellanox and NVIDIA. The papers and presentations are available [**here**]. http://www.csm.ornl.gov/OpenSHMEM2014/

WACPAD14 Workshop at SC'14

Oscar Hernandez

Oscar Hernandez organized the first international workshop on high-level directives to program accelerators. The workshop had a strong participation with more than 20 papers submitted and 7 papers accepted (23% acceptance rate). The workshop was co-located with Supercomputing 2014.

The goal of this workshop was to bring together users, vendors, and tools providers to share their knowledge and experiences to program heterogeneous systems using directive-based programming interfaces such as OpenACC, OpenMP, etc to achieve good performance. The workshop emphasized the future direction of accelerator programming using directives and how researchers can address better the user and tools-ecosystem needs.

http://www.openacc.org/WACCPD14

Workshop on Advanced Modeling and Simulation for Additive Manufacturing

Sreekanth Pannala, B. Radhakrishnan (Rad), Suzy Tichenor, Srdjan Simunovic, and Sarma Gorti

On November 4-5, 2014, a workshop was organized at Oak Ridge National Laboratory to discuss challenges and opportunities for advanced modeling and simulation to augment and accelerate progress in the rapidly developing field of additive manufacturing (AM). It is widely-

acknowledged that the rapid advances in AM have the potential to dramatically transform the manufacturing industry. However, improvements in performance and consistency of material properties, optimized process control, reduced tolerances, and new materials and processes are required in order for AM to meet performance, quality and cost targets, along with increased manufacturing speed.

There were 61 attendees, representing private industry, academia, DOE national laboratories, and other U.S. government agencies. Approximately ⅓ of the participants were from industry, and represented both practitioners using (or planning to use) AM in production and independent software vendors (ISVs) developing and deploying tools for modeling and simulation of AM processes.

UPCOMING

ASCR Workshop on Quantum Computing for Science (Feb. 17-18)

Travis Humble

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

http://www.csm.ornl.gov/workshops/ascrqcs2015/

International Workshop on The Lustre Ecosystem: Challenges and Opportunities (March 3-4)

Neena Imam, Mike Brimm, Oral Sarp

In this workshop, we seek contributions that explore improvements in the performance and flexibility of the Lustre file system for supporting diverse workloads. This will be a great opportunity for the Lustre community to discuss the challenges associated with enhancing Lustre for diverse applications, the technological advances necessary, and the associated ecosystem.

Specific topics of interest include, but are not limited to:

- Workload Characterization
- Adaptability and scalability of Lustre for diverse workloads
- Resilience and Serviceability of Lustre
- Knowledge Provenance in Lustre
- Application-driven Lustre Benchmarking
- Integrating Big Data Technologies with Lustre
- Performance Monitoring Tools for Lustre

http://lustre.ornl.gov/ecosystem/

Numerical and Computational Developments to Advance Multiscale Earth System Models (MSESM) (June 1-13)

Kate Evans

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

Topics include, but are not limited to:

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

http://www.csm.ornl.gov/iccs/index.html

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

Clayton Webster

The special issues workshop will feature original work by leading researchers in numerical analysis, mathematical modeling and computational science. Guest editors will select and invite the contributions. The papers will undergo rigorous peer review process managed by the guest editors (Bochev, Du, Hou and Webster) and supervised by the journal's Editor-in-Chief, Prof. Leszek Demkowicz. This work will then appear is a special issue of the journal Computers and Mathematics with Application. We anticipate receiving submissions covering the following subject areas:

- Climate modeling and groundwater flows: including ocean and ice sheet modeling, numerical algorithms
- Computational fluid dynamics

Events (continued)

- Computational geometry, mesh generation and image processing
- Finite element methods: including Least-squares FEMs, Stabilized FEMs,
- Compatible FEMs, DG, and DPG
- Flow control, theory, numerical methods and applications
- Materials modeling: including multi-scale methods, quasi-continuum
- methods, atomistic to continuum coupling, peridynamics and nonlocal model, applications in superconductivity
- Reduced order modeling, domain decomposition and multidisciplinary
- simulation and optimization
- UQ and numerical methods for partial differential equations with random inputs

http://www.csm.ornl.gov/workshops/ASCAM/index.html

CAM Seminar Series

Pablo Seleson

The Computer Science and Mathematics Division (CSMD) holds the Computational & Applied Mathematics (CAM) seminar series, with weekly presentations from researchers within the CSMD and other divisions at ORNL, as well as from external speakers. The CAM seminar brings together researchers who share common interests in the use of mathematical and computational models and tools to solve scientific and engineering problems.

- January 13 - Dr. Zhiwen Zhang
- January 15 - Dr. Ke Shi
- January 20 - Dr. Lin Mu
- January 22 - Dr. Masayuki Yano
- January 29 - Dr. Yehuda Braiman
- February 3 - Mr. David Witman
- February 3 - Mr. Lukas Bystricky
- February 12 - Dr. Feng Bao
- February 19 - Dr. Tadele Mengesha
- February 27 - Dr. Jichun Li
- March 5 - Dr. Yulong Xing
- March 12 - Dr. Guannan Zhang
- March 19 - Dr. Eirik Endeve
- March 26 - Garrett E. Granroth

http://cam.ornl.gov/seminars.html

Community Service

- David E. Bernholdt, Program Committee, First International Workshop on Hardware-Software Co-Design for High-Performance Computing (Co-HPC 2014)
- David E. Bernholdt, Program Committee, Workshop on Accelerator Programming Using Directives (WACCPD)
- David E. Bernholdt, Program Committee, International Parallel and Distributed Processing Symposium (IPDPS 2015)
- David E. Bernholdt, Reviewer, DOE Office of Science Advanced Scientific Computing Research (ASCR) Small Business Innovation Research (SBIR) Program
- David E. Bernholdt, Reviewer, ORAU/ORNL High Performance Computing Grant Program
- Christian Engelmann, technical program committee member, 23rd Euromicro International Conference on Parallel, Distributed and network-based Processing (PDP), Turku, Finland, March 6-8, 2015
- Christian Engelmann, technical program committee member, 15th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid)
- 2015, Shenzhen, Guangdong, China, May 4-7, 2015
- Manjunath Gorentla Venkata, Co-chair, OpenSHMEM User Group 2014, Eugene, Oregon
- Tomislav Janjusic, reviewer, First International Workshop on Hardware-Software Co-design for High Performance Computing, 2014
- Christos Kartsaklis, technical program committee member, 23rd Euromicro International Conference on Parallel, Distributed and network-based Processing (PDP)
- Christos Kartsaklis, program committee, Special Session on High Performance Computing in Modelling and Simulation (HPCMS), within the 23rd Euromicro International Conference on Parallel, and Network-Based Computing (PDP 2015)
- Christos Kartsaklis, program committee, First International Workshop on Hardware-Software Co-Design for High Performance Computing (Co-HPC 2014), in conjunction with SC14: The International Conference for High Performance Computing, Networking, Storage, and Analysis
- Christos Kartsaklis, program committee, WACCPD 2014 : Workshop on accelerator programming using directives (WACCPD14), in conjunction with SC14: The International Conference for High Performance Computing, Networking, Storage, and Analysis
- Christos Kartsaklis, track chair, Ubiquitous Communications, 13th IEEE International Conference on Ubiquitous Computing and Communications (IUCC 2014) Christos Kartsaklis, program committee, 28th

Community Service [Continued]

GI/ITG International Conference on Architecture of Computing Systems (ARCS'2015)

- Tiffany M. Mintz, recruiting, Grace Hopper Conference 2014
- Sparsh Mittal, Reviewer for ACM Transactions on Architecture and Code Optimization
- Sarah Powers, reviewer, Parallel Computing
- Pavel Shamis, Program Committee Member / Organizer, OpenSHMEM User Group 2014, Eugene, Oregon

SC 2014

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.

SC Planning Committee

- Christian Engelmann: Posters Committee Member
- Qing Gary Liu: Technical Papers - Committee Member - Data Analytics, Visualization & Storage
- Arthur Maccabe: Technical Papers - Committee Member - Systems Software
- David Pugmire: Scientific Visualization and Data Analytics Showcase Committee Member
- Philip C. Roth: Signage Chair, SC14 BoF Committee Adviser, Posters Committee Member
- Jeffrey Vetter: Technical Program Deputy Chair, ACM Gordon Bell Prize Committee Member, Emerging Technologies Co-Chair, Emerging Technologies Committee Member

The following is a list of the Workshops, Tutorials, BOFs, and Paper sessions in which CSMD's researchers took part.

- 5TH SC WORKSHOP ON BIG DATA ANALYTICS: CHALLENGES AND OPPORTUNITIES: Ranga Raju Vatsavai - Oak Ridge National Laboratory, Scott Klasky - Oak Ridge National Laboratory and Manish Parashar - Rutgers University
- DISCS-2014: INTERNATIONAL WORKSHOP ON DATA INTENSIVE SCALABLE COMPUTING SYSTEMS: Philip C. Roth - Oak Ridge National Laboratory, Weikuan Yu - Auburn University and Yong Chen - Texas Tech University
- SCALING I/O BEYOND 100,000 CORES USING ADIOS: Norbert Podhorszki, Scott Klasky and Qing Liu
- INTRODUCING R: FROM YOUR LAPTOP TO HPC AND BIG DATA: George Ostrouchov and Drew Schmidt
- 5TH WORKSHOP ON LATEST ADVANCES IN SCALABLE ALGORITHMS FOR LARGE-SCALE SYSTEMS (SCALA): Vassil Alexandrov - Barcelona Supercomputing Center, Al Geist - Oak Ridge National Laboratory and Christian Engelmann - Oak Ridge National Laboratory
- WACCPD: FIRST WORKSHOP ON ACCELERATOR PROGRAMMING USING DIRECTIVES: Sunita Chandrasekaran - University of Houston, Oscar Hernandez - Oak Ridge National Laboratory and Fernanda Foertter - Oak Ridge National Laboratory
- EFFECTIVE HPC VISUALIZATION AND DATA ANALYSIS USING VISIT: David Pugmire
- INTRODUCTORY AND ADVANCED OPENSHMEM PROGRAMMING: Tony Curtis, Swaroop Pophale, Oscar Hernandez, Pavel Shamis, Dounia Khaldi and Aaron Welch
- INFINICORTEX: CONCURRENT SUPERCOMPUTING ACROSS THE GLOBE UTILIZING TRANS-CONTINENTAL INFINIBAND AND GALAXY OF SUPERCOMPUTERS: Marek Michalewicz, Yuefan Deng, Tin Wee TAN, Yves Poppe, Scott Klasky and David Southwell
- LUSTRE COMMUNITY BOF: AT THE HEART OF HPC AND BIG DATA: Galen Shipman (Primary Session Leader) - Oak Ridge National Laboratory and Hugo Falter (Secondary Session Leader) - European Open File System
- OPERATING SYSTEM AND RUN-TIME FOR EXASCALE: Marc Snir (Primary Session Leader) - Argonne National Laboratory, Arthur Maccabe (Secondary Session Leader) - Oak Ridge National Laboratory and John Kubiatowicz (Secondary Session Leader) - University of California, Berkeley
- BEST PRACTICES AND LESSONS LEARNED FROM DEPLOYING AND OPERATING LARGE-SCALE DATA-CENTRIC PARALLEL FILE SYSTEMS: Mark Gary (Chair) - Lawrence Livermore National Laboratory, Sarp Oral - Oak Ridge National Laboratory, James Simmons - Oak Ridge National Laboratory, Jason Hill - Oak Ridge National Laboratory, Dustin Leverman - Oak Ridge National Laboratory, Feiyi Wang - Oak Ridge National Laboratory, Matthew Ezell - Oak Ridge National Laboratory, Ross Miller - Oak Ridge National Laboratory, Douglas Fuller - Oak Ridge National Laboratory, Raghul Gunasekaran - Oak Ridge National Laboratory, Youngjae Kim - Oak Ridge National Laboratory, Saurabh Gupta - Oak Ridge National Laboratory, Devesh Tiwari - Oak Ridge National Laboratory, Sudharshan Vazhkudai - Oak Ridge National Laboratory, James Rogers - Oak Ridge National Laboratory, David Dillow - Self Employed, Arthur S. Bland - Oak Ridge National Laboratory and Galen M. Shipman - Oak Ridge National Laboratory
- CHANGING OPERATING SYSTEMS IS HARDER THAN CHANGING PROGRAMMING LANGUAGES: Arthur B. Maccabe (Moderator) - Oak Ridge National Laboratory, Marc Snir - Argonne National Laboratory, Pete Beckman - Argonne National Laboratory, Patrick Bridges - University of New Mexico, Ron Brightwell - Sandia National Laboratories, Orran Krieger - Boston University, John Kubiatowicz - University of California, Berkeley, Matsuoka Satoshi - Tokyo Institute of Technology Hanck Hoffman - University of Chicago

Community Service [Continued]

- INFINICORTEX: CONCURRENT SUPERCOMPUTING ACROSS THE GLOBE UTILIZING TRANS-CONTINENTAL INFINIBAND AND GALAXY OF SUPERCOMPUTERS: Marek Michalewicz, Yuefan Deng, Tin Wee TAN, Yves Poppe, Scott Klasky and David Southwell
- GREATER THAN 10X ACCELERATION OF FUSION PLASMA EDGE SIMULATIONS USING THE PARAREAL ALGORITHM: Debasmita Samaddar - Culham Centre for Fusion Energy /UK Atomic Energy Authority, David P. Coster - Max Planck Institute of Plasma Physics, Xavier Bonnin - National Center for Scientific Research
- Christoph Bergmeister - University of Innsbruck, Eva Havlickova - Culham Centre for Fusion Energy/UK Atomic Energy Authority, Wael R. Elwasif - Oak Ridge National Laboratory, Lee A. Berry - Oak Ridge National Laboratory and Donald B. Batchelor - Oak Ridge National Laboratory
- LESSONS FROM ANALYZING FAN-IN COMMUNICATIONS: Terry Jones - Oak Ridge National Laboratory
- A FRAMEWORK FOR ANALYZING THE COMMUNITY LAND MODEL WITHIN THE COMMUNITY EARTH SYSTEM MODELS: Dali Wang - Oak Ridge National Laboratory, Wei Wu - University of Tennessee, Yang Xu - University of Tennessee, Tomislav Janjusic - Oak Ridge National Laboratory, Wei Ding - Oak Ridge National Laboratory, Frank Winkler - Oak Ridge National Laboratory, Nick Forrington - Oak Ridge National Laboratory and Oscar Hernandez - Oak Ridge National Laboratory
- INTEGRATED OPTIMIZATION OF PERFORMANCE, POWER AND RESILIENCE FOR EXTREME SCALE SYSTEMS: Dong Li (Primary Session Leader) - Oak Ridge National Laboratory and Kathryn Mohror (Secondary Session Leader) - Lawrence Livermore National Laboratory
- QUANTITATIVELY MODELING APPLICATION RESILIENCY WITH THE DATA VULNERABILITY FACTOR: Ananta Tiwari (Chair) - PMaC Lab, SDSC, Li Yu - Illinois Institute of Technology, Dong Li - Oak Ridge National Laboratory, Sparsh Mittal - Oak Ridge National Laboratory and Jeffery S. Vetter - Oak Ridge National Laboratory
- OPENSHMEM: FURTHER DEVELOPING THE SHMEM STANDARD FOR THE HPC COMMUNITY: Tony Curtis (Primary Session Leader) - University of Houston, Steve Poole (Secondary Session Leader) - Department of Defense, and Oscar Hernandez (Secondary Session Leader) - Oak Ridge National Laboratory
- SUPER-R: SUPERCOMPUTING AND R FOR DATA-INTENSIVE ANALYSIS: Weijia Xu (Primary Session Leader) - University of Texas at Austin, Hui Zhang (Secondary Session Leader) - Indiana University and George Ostrouchov (Secondary Session Leader) - Oak Ridge National Laboratory
- EXPERIENCING HPC FOR UNDERGRADUATES: CAREERS IN HPC: Jeffrey K. Hollingsworth (Chair) - University of Maryland, David Bernholdt - Oak Ridge National Laboratory, Brad Chamberlain - Cray Inc., Elizabeth R. Jessup - University of Colorado, Rob Schreiber - Hewlett-Packard Development Company, L.P. and Michela Taufer - University of Delaware
- EVOLVING HPC SOFTWARE ECOSYSTEM FOR EMERGING NON-VOLATILE MEMORY TECHNOLOGIES: Dong Li (Primary Session Leader) - Oak Ridge National Laboratory, Sparsh Mittal (Secondary Session Leader) - Oak Ridge National Laboratory and Jeffrey Vetter (Secondary Session Leader) - Oak Ridge National Laboratory
- EXPLORING AUTOMATIC, ONLINE FAILURE RECOVERY FOR SCIENTIFIC APPLICATIONS AT EXTREME SCALES: Patrick Bridges (Chair) - University of New Mexico, Marc Gamell - Rutgers University, Daniel S. Katz - University of Chicago and Argonne National Laboratory, Hemanth Kolla - Sandia National Laboratories, Jacqueline Chen - Sandia National Laboratories, Scott Klasky - Oak Ridge National Laboratory and Manish Parashar - Rutgers University

Awards and Recognition

ORNL Awards Night

Research Accomplishment

Andrew Godfrey, Roscoe Bartlett, Kursat Bekar, Cihangir Celik, Thomas Evans, Gregory Davidson, Steven Hamilton, Wayne Joubert, Seth Johnson, Tara Pandya

For outstanding research accomplishment in the simulation of the AP1000 advanced light water reactor that brings a new high-performance modeling and simulation capability from R&D to industrial deployment and application, representing a primary achievement for CASL.

CSMD Awards

Most Distinguished Scientific Paper

Paul Kent

The vibrations of ions in solids at finite temperature depend on interatomic force–constants that result from electrostatic interactions between ions, and the response of the electron density to atomic displacements. At high temperatures, vibration amplitudes are substantial, and electronic states are affected, thus modifying the screening properties of the electron density. By combining inelastic neutron scattering measurements of Fe1-xCoxSi as a function of temperature, and finite-temperature first-principles calculations including thermal disorder effects, we show that the coupling between phonons and electronic structure results in an anomalous temperature dependence of phonons. The strong concomitant

Awards and Recognition [Continued]

renormalization of the electronic structure induces the semiconductor-to-metal transition that occurs with increasing temperature in FeSi. Our results show that for systems with rapidly changing electronic densities of states at the Fermi level, there are likely to be significant phonon–electron interactions, resulting in anomalous temperature-dependent properties.

Olivier Delaire, Karol Marty, Matthew B. Stone, Paul R. C. Kent, Matthew S. Lucas, Douglas L. Abernathy, David Mandrus, and Brian C. Sales (2011), Phonon softening and metallization of a narrow-gap semiconductor by thermal disorder, Proc. Nat. Acad. Sci., 108(12), 4725–4730

http://www.pnas.org/content/108/12/4725.full

Most Distinguished Award for Software

Gonzalo Alvarez

DMRG++ framework, enabling researchers to gain critical new insights into phase transitions in spin systems, and strongly correlated electron models of transition metal oxides

Most Distinguished Award for a Special Contribution

Eric Lingerfelt

Computational Infrastructure for Nuclear Astrophysics (CINA) cloud-based software as a service system for modeling nuclear reaction processes, available at nucastrodata.org

Significant Event Awards

- Clayton Webster and Guannan Zhang – "Stochastic finite element methods for PDEs with random input data" review article published.
- Galen Shipman, Marcia Branstetter, Brian Jewell, Ben Mayer, John Quigley, Chad Steed, John Harney,
- Brian Smith, Peter Thornton, and Kate Evans – Successful completion of Accelerated Climate Model for Energy (ACME) workflow & data analysis demonstration.
- Thomas Maier, Michael Summers, and Thomas Schulthess – Transformative Developments in Time to Solution for Simulations of High-Tc Superconductors.
- Benjamin Preston, Thomas Willbanks, Peter Thornton, Forrest Hoffman, Steven Fernandez, Xiaoying Shi,
- Jaifu Mao, Sherry Wright, Brett Hopwood, Paul Hanson, Viginia Dale, and Pat Worley – Intergovernmental Panel on Climate Change & National Climate Assessment Work.
- Peter Thornton, Pat Worley, Forrest Hoffman, Jim Hack, and Kate Evans – Successful completion of ACME Strategy, Proposal, & Review for DOE BER Office .
- ay Jay Billings, Jordan Deyton, Anna Wojtowicz, Taylor Patterson, Alex McCaskey – ICE Accepted as ORNL's First Eclipse Project & Released with Comprehensive Support for NEAMS Product Lines.
- Paul Kent – Energy Dissipation to Defect Evolution (EDDE).
- Guruprasad Kora – Adaptive Biosystems Imaging Proposal.

Professional Societies and Activities

Bobby Sumpter:

- Elected Fellow of the American Physical Society (APS) for outstanding scientific impact and development in computational soft matter and nanoscience through the development and use of principles from computer science and mathematics and the results of theoretical physics and chemistry to facilitate solving materials problems and discovery of new functional materials

Clayton Webster:

- Elected as Program Director for SIAM UQ-SIAG (2 year term, starting 01/15)
- Elected member of SIAM Academic/Industrial Council (3 year term starting 01/15)
- Appointed Co-Chair of SIAM UQ16 Conference in Lausanne, Switzerland (04/16)

Publications and Presentations

Abstract - conference

- Brooks, Richard R (Clemson University), Wu, Qishi (University of Memphis), Sen, Satyabrata (ORNL); Efficient Network Detection of Radiation Sources Using Localization; IEEE Nuclear Science Symposium, Seattle, Washington, 11/2014
- Evans, Katherine J. (ORNL), Jiang, Tianyu NMI (ORNL), Deng, Yi (Georgia Institute of Technology, Atlanta); Diagnosing the connections between western US extreme precipitation and remote forcing; AGU, San Fransisco, California, 12/2014
- Mintz, Tiffany M. (ORNL), Hernandez, Oscar R. (ORNL), Bernholdt, David E. (ORNL); Transitioning To A New HPC Programming Paradigm; Grace Hopper Celebration of Women in Computing, Phoenix, Arizona, 10/2014
- Sumpter, Bobby G. (ORNL); Interfacial Dynamics in Polymer-Based Multicomponent Materials; Louisiana State University, 12/2014
- Tian, Chong (ORNL), Chan, Ki Shing (Chinese University of Hong Kong (CUHK)), Morales, Allan (George Washington University), Wong, Kwai (ORNL); Runtime Systems and Out-of-Core Cholesky Factorization on

Publications and Presentations [Continued]

the Intel Xeon Phi System; The 15th International Conference on Parallel and Distributed Computing, Applications and Technologies, Hong Kong, , 12/2014

- Turner, John A. (ORNL), Allu, Srikanth (ORNL), Elwasif, Wael R. (ORNL), Kalnaus, Sergiy (ORNL), Pannala, Sreekanth (ORNL), Simunovic, Srdjan (ORNL); Toward Predictive Crash Modeling of Automotive Batteries (abstract); Battery Safety 2014, Washington, District of Columbia, 11/2014

Book chapter or article

- Kumar, Rajeev (ORNL), Goswami, Monojoy (ORNL), Carrillo, Jan-Michael Y. (ORNL), Sumpter, Bobby G. (ORNL); Insights obtained from modeling of organic photovoltaics: morphology, interfaces and coupling with charge transport; Organic Solar Cells: Materials, Devices, Interfaces, and Modeling, 10/2014

Journal article

- Guy, Robert (University of California, Davis), Philip, Bobby (ORNL), Griffith, Boyce (New York University); Geometric Multigrid for an Implicit-time Immersed Boundary Method; Advances in Computational Mathematics, 10/2014
- He, Yadong (Virginia Tech), Huang, Jingsong (ORNL), Sumpter, Bobby G. (ORNL), Kornyshev, Alexei (Imperial College London), Qiao, Rui (ORNL); Dynamic Charge Storage in Ionic Liquids-filled Nanopores: Insights from a Computational Cyclic Voltammetry Study; Journal of Physical Chemistry Letters, 12/2014
- Kapnick, Sarah (NOAA Geophysical Fluid Dynamics Laboratory (GFDL), Princeton, NJ), Delworth, Tom (NOAA Geophysical Fluid Dynamics Laboratory (GFDL), Princeton, NJ), Ashfaq, Moetasim (ORNL), Malyshev, Sergey (NOAA Geophysical Fluid Dynamics Laboratory (GFDL), Princeton, NJ), Milley, P.C.D (United States Geological Service (USGS)); Snowfall less sensitive to warming in Karakoram than in Himalayas due to a unique seasonal cycle; Nature Geoscience, 10/2014
- Liang, Liangbo (Rensselaer Polytechnic Institute (RPI)), Lin, Wenzhi (ORNL), Wang, Jun (ORNL), Sumpter, Bobby G. (ORNL), Meunier, Vincent (Rensselaer Polytechnic Institute (RPI)), Pan, Minghu (ORNL); Electronic Bandgap and Edge Reconstruction in Phosphorene Materials; Nano Letters, 11/2014
- Liu, Ying (Clemson University), Huxtable, Scott T (Virginia Polytechnic Institute and State University), Yang, Bao (University of Maryland), Sumpter, Bobby G. (ORNL), Qiao, Rui (Clemson University); Nonlocal Thermal Transport across Embedded Few-Layer Graphene Sheets; Journal of Physics: Condensed Matter, 11/2014
- Mittal, Sparsh (ORNL), Zhang, Zhao (Iowa State University); EnCache: A Dynamic Profiling Based Reconfiguration Technique for Improving Cache Energy Efficiency; Journal of Circuits, Systems, and Computers, 12/2014
- Williams, Brian P. (ORNL), Humble, Travis S. (ORNL), Grice, Warren P. (ORNL); Nonlocal polarization interferometer for entanglement detection; Physical Review A, 10/2014

LDRD report

- Brim, Michael J. (ORNL), Cao, Qing (University of Tennessee, Knoxville (UTK)), Jones, Terry R. (ORNL), Oral, H Sarp (ORNL), Yu, Weikuan (Auburn University, Auburn, Alabama), Wang, Teng (Auburn University, Auburn, Alabama), Wan, Lipeng (ORNL), Wang, Feiyi (ORNL); 6565 - Towards a Scalable and Resilient Infrastructure for Big Data
- Leuze, Michael Rex (ORNL), Uberbacher, Edward C. (ORNL), Boehnen, Chris Bensing (ORNL), Emmons, Alexandra L. (ORNL), Figueroa-Soto, Cristina (ORNL); DNA2Face: Predicting Faces from a DNA Sample
- Stoyanov, Miroslav K. (ORNL); Algorithm Resilience with Respect to Hardware Error

Letter report

- McCaskey, Alex (ORNL), Bennett, Andrew R. (ORNL), Billings, Jay Jay (ORNL); Enhancements to the SHARP Build System and NEK5000 Coupling; 10/2014

ORNL report

- Lu, Dan (ORNL), Zhang, Guannan (ORNL), Webster, Clayton G. (ORNL), Barbier, Charlotte N. (ORNL); A multilevel Monte Carlo approach for predicting the uncertainty in oil reservoir simulations; 11/2014
- Mittal, Sparsh, Poremba, Matthew, Vetter, Jeffrey, Xie, Yuan; “Exploring Design Space of 3D NVM and eDRAM Caches Using DESTINY Tool”, Oak Ridge National Laboratory, Technical Report number ORNL/TM-2014/636, 2014.

Other

- Patterson, Taylor C. (ORNL), Wojtowicz, Anna (ORNL), Deyton, Jordan H. (ORNL), McCaskey, Alex (ORNL),

Publications and Presentations (Continued)

Billings, Jay Jay (ORNL); Modeling and Simulation Made NiCE with the Eclipse Platform; 10/2014

Paper in conference proceedings (book, CD)

- Campbell, Stuart I. (ORNL), Kohl, James Arthur (ORNL), Granroth, Garrett E. (ORNL), Miller, Ross G. (ORNL), Doucet, Mathieu (ORNL), Stansberry, Dale V. (ORNL), Proffen, Thomas E. (ORNL), Taylor, Russell J. (ORNL), Dillow, David (None); Accelerating Data Acquisition, Reduction, and Analysis at the Spallation Neutron Source; The 10th IEEE International Conference on e-Science, Guaruji, Brazil, 10/2014
- Combs, J.; Nazor, J.; Thysell, R.; Santiago, F.; Hardwick, R. M.; Olson, L.; Rivoire, S.; Hsu, C.; Poole, S.W.; Power Signatures of High-Performance Computing Workloads. In the Proceedings of the 2nd International Workshop on Energy Efficient Supercomputing (E2SC), November 2014.
- Engelmann, Christian (ORNL), Naughton, III, Thomas J. (ORNL); Improving the Performance of the Extreme-scale Simulator; 18th IEEE/ACM International Symposium on Distributed Simulation and Real Time Applications (DS-RT) 2014, Toulouse, France, 10/2014
- Habermann, Ted E. (ORNL), Billings, Jay Jay (ORNL); The Hierarchical Data Format (HDF): A Foundation for Sustainable Data and Software; Working Towards Sustainable Software for Science: Practice and Experiences, New Orleans, Louisiana, 11/2014
- Lagadapati, Mahesh (North Carolina State University), Mueller, Frank (North Carolina State University), Engelmann, Christian (ORNL); Tools for Simulation and Benchmark Generation at Exascale; 7th Parallel Tools Workshop, Dresden, Germany, 10/2013
- Mittal, Sparsh (ORNL), Vetter, Jeffrey S. (ORNL); EqualChance: Addressing Intra-set Write Variation to Increase Lifetime of Non-volatile Caches; 2nd USENIX Workshop on Interactions of NVM/Flash with Operating Systems and Workloads (INFLOW), Broomsfield, Colorado, 10/2014
- Powers, Sarah S. (ORNL), Sukumar, Sreenivas R. (ORNL); Defining “normal”: metrics for mining heterogeneous graphs at large scales; 2014 INFORMS Workshop on Data Mining and Analytics (DMA 2014), San Francisco, California, 11/2014
- Powers, Sarah; “A Study of the Impact of Scheduling Parameters in Heterogeneous Computing Environments,” in Proc. of 2014
- Winter Simulation Conference (WSC 2014), Savannah, GA, December 2014.
- Rao, Nageswara S. (ORNL); On Undecidability Aspects of Resilient Computations and Implications to Exascale; Euro-Par 2014: Parallel Processing Workshops: Resilience 2014, Porto, Portugal, 11/2014
- Sreepathi, Sarat (ORNL), Grodowitz, Megan L. (ORNL), Lim, Robert V. (ORNL), Taffet, Philip A. (ORNL), Roth, Philip C. (ORNL), Meredith, Jeremy S. (ORNL), Lee, Seyong (ORNL), Li, Dong (ORNL), Vetter, Jeffrey S. (ORNL); Application Characterization using Oxbow Toolkit and PADS Infrastructure; First International Workshop on Hardware-Software Co-Design for High Performance Computing (Co-HPC 2014), In conjunction with SC-14, New Orleans, Louisiana, 11/2014

Presentation material - conference

- Bernholdt, David E. (ORNL); Planning for change:Designing large-scale software systems for emerging HPC environments; 248th American Chemical society National Meeting, San Francisco, California
- Dai, Hongwen; Kartsaklis, Christos; Li, Chao; Janjusic, Tomislav; Zhou, Huiyang; RACB: Resource Aware Cache Bypass on GPUs, in 5th Workshop on Applications for Multi-Core Architectures, Held in conjunction with the 26th International Symposium on Computer Architecture and High Performance Computing (SBAC-PAD 2014), 2014.
- Hao, Pengfei; Shamis, Pavel; Gorentla Venkata, Manjunath; Pophale, Swaroop; Welch, Aaron; Poole, Stephen W.; Chapman, Barbara; “Fault Tolerance for OpenSHMEM”, OpenSHMEM Users Group (OUG 2014), 2014.
- Huang, Zhuoyi; Rustagi, Navin; Veeraraghavan, Narayanan; Carroll, Andrew; Xue1, Cheng; Metcalf, Ginger A.; Gorentla Venkata, Manjunath; Kalra, Divya; Cupples, L. Adrienne; Muzny, Donna; Gibbs, Richard; Boerwinkle, Eric; Yu, Fuli; “gSNAP: An ensemble variant calling approach in >5,000 low coverage whole genomes”. Poster, CHARGE PI Meeting, Washington DC, 2014.
- Janjusic, Tomislav; Shamis, Pavel; Gorentla Venkata, Manjunath; Poole, Stephen W.; “OpenSHMEM Reference Implementation using UCCS-uGNI Transport Layer”, OpenSHMEM Users Group (OUG 2014), 2014.
- Jones, Terry R. (ORNL), Settlemyer, Bradley W. (ORNL); Lessons From Analyzing Fan-In Communications; The

Publications and Presentations (Continued)

27th International Conference for High Performance Computing, Networking, Storage and Analysis (SC'14), New Orleans, Louisiana

- Lingerfelt, Eric; "Accelerating Scientific Discovery with the Bellerophon Software System", ORNL CSMD Seminar, Nov. 13, 2014.
- Mittal, Sparsh (ORNL); "EqualChance: Addressing Intra-set Write Variation to Increase Lifetime of Non-volatile Caches", USENIX INFLOW workshop at Broomfield, CO, 2014
- Ostrouchov, George (ORNL); pbdR: A Sustainable Path for Scalable Statistical Computing; HPTCDL - First Workshop for High Performance Technical Computing in Dynamic Languages, held in conjunction with SC14: The International Conference on High Performance Computing, Networking, Storage and Analysis, New Orleans, Louisiana
- Patterson, Taylor C. (ORNL), Billings, Jay Jay (ORNL); Take a Look at This: Visualizations for Simulation Results in Eclipse; EclipseCon Europe 2014, Ludwigsburg, Germany
- Powers, Sarah S. (ORNL); Enhancing HPC Scheduling through Predictive Analytics; INFORMS 2014, San Francisco, California
- Powers, Sarah; " 'Big data' graph mining as a tool for fraud detection", Grace Hopper Conference, Phoenix, AZ, October 9, 2014.
- Shamis, Pavel (ORNL), Gorentla Venkata, Manjunath (ORNL), Poole, Stephen W. (ORNL), Tony, Curtis (University of Houston, Houston), Welch, Donald A. (ORNL); Evaluation of the Universal Common Communication Substrate (UCCS) with OpenSHMEM; Super Computing 2013, Denver, Colorado
- Shamis, Pavel; Pophale, Swaroop; Gorentla Venkata, Manjunath; Poole, Stephen W.; Dubman, Michael; Graham, Richard; Goldenberg, Dror; Shainer, Gilad; "Development and Extension of Atomic Memory Operations in OpenSHMEM", OpenSHMEM Users Group (OUG 2014), 2014.
- Turner, John A. (ORNL), Allu, Srikanth (ORNL), Elwasif, Wael R. (ORNL), Kalnaus, Sergiy (ORNL), Kumar, Abhishek (ORNL), Pannala, Sreekanth (ORNL), Simunovic, Srdjan (ORNL), Wang, Hsin (ORNL); Toward Predictive Crash Modeling of Automotive Batteries; Battery Safety 2014, Washington, District of Columbia
- Wang, Dali; Wu, Wei; Xu, Yang; Janjusic, Tomislav; Ding, Wei; Winkler, Frank; Forrington, Nick; Hernandez, Oscar; A Framework for Analyzing the Community Land Model within the Community Earth System Models, poster, International Conference for High Performance Computing, Networking, Storage and Analysis (SC2014), 2014.
- Welch, Aaron; Pophale, Swaroop, Shamis; Pavel, Hernandez, Oscar; Poole, Stephen; Chapman, Barbara; "Extending the OpenSHMEM Memory Model to Support User-Defined Spaces", 8th International Conference on Partitioned Global Address Space Programming Models (PGAS 2014), 2014.

Presentation material - no conference

- Lynch, Vickie E. (ORNL), Borreguero Calvo, Jose M. (ORNL), Hagen, Mark E. (ORNL), Proffen, Thomas E. (ORNL), Shipman, Galen M. (ORNL), Sumpter, Bobby G. (ORNL), Delaire, Olivier A. (ORNL); SNS Workflow Overview
- Patterson, Taylor C. (ORNL), Billings, Jay Jay (ORNL); Take a Look at This: Visualizations for Simulation Results in Eclipse
- Turner, John A. (ORNL); Coupled Physics and the Virtual Environment for Reactor Applications (VERA)
- Turner, John A. (ORNL); Welcome and Overview of ORNL and CASL

About CSMD

The Computer Science and Mathematics Division (CSMD) is ORNL's premier source of basic and applied research in high-performance computing, applied mathematics, and intelligent systems. Basic and applied research programs are focused on computational sciences, intelligent systems, and information technologies.

Our mission includes working on important national priorities with advanced computing systems, working cooperatively with U.S. industry to enable efficient, cost-competitive design, and working with universities to enhance science education and scientific awareness. Our researchers are finding new ways to solve problems beyond the reach of most computers and are putting powerful software tools into the hands of students, teachers, government researchers, and industrial scientists.

The Division is composed of nine Groups. These Groups and their Group Leaders are:

- Complex Systems – Jacob Barhen
- Computational Biomolecular Modeling & Bioinformatics – Mike Leuze
- Computational Chemical and Materials Sciences – Bobby Sumpter
- Computational Earth Sciences – Kate Evans
- Computational Engineering and Energy Sciences – John Turner
- Computational Applied Mathematics – Clayton Webster
- Computer Science Research – David Bernholdt
- Future Technologies – Jeff Vetter
- Scientific Data – Scott Klasky

About this Newsletter

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

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

Contact Information

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Technical Communications - Daniel Pack - packdl@ornl.gov

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