Safer Batteries through Coupled Multiscale Modeling

John Turner, Srikanth Allu, Mark Berrill, Wael Elwasif, Sergiy Kalnaus, Abhishek Kumar, Damien Lebrun-Grandie, Sreekanth Pannala, and Srdjan Simunovic

Batteries are highly complex electrochemical systems, with performance and safety governed by coupled nonlinear electrochemical-electrical-thermal-mechanical processes over a range of spatiotemporal scales. We describe a new, open source computational environment for battery simulation known as VIBE - the Virtual Integrated Battery Environment. VIBE includes homogenized and pseudo-2D electrochemistry models such as those by Newman-Tiedemann-Gu (NTG) and Doyle-Fuller-Newman (DFN, a.k.a. DualFoil) as well as a new advanced capability known as AMPERES (Advanced MultiPhysics for Electrochemical and Renewable Energy Storage). AMPERES provides a 3D model for electrochemistry and full coupling with 3D electrical and thermal models on the same grid. VIBE/AMPERES has been used to create three-dimensional battery cell and pack models that explicitly simulate all the battery components (current collectors, electrodes, and separator). The models are used to predict battery performance under normal operations and to study thermal and mechanical response under adverse conditions.

This work was performed at ORNL and sponsored by DOE’s EERE office.
Science Highlights [Continued]

Scalable and Fault Tolerant Failure Detection and Consensus

A. Katti, G. Di Fatta, T. Naughton, and C. Engelmann

Future extreme-scale high-performance computing systems will be required to work under frequent component failures. The MPI Forum’s User Level Failure Mitigation proposal has introduced an operation (MPI_Commm_shrink) to synchronize the alive processes on the list of failed processes, so that applications can continue to execute even in the presence of failures by adopting algorithm-based fault tolerance techniques. The MPI_Comm_shrink operation requires a fault tolerant failure detection and consensus algorithm. This work developed two novel failure detection and consensus algorithms to support this operation. The algorithms are based on Gossip protocols and are inherently fault-tolerant and scalable. The first algorithm is based on global knowledge: each process maintains a local view of the entire system state to achieve consensus on failed processes. A Gossip protocol is used to detect failures and to exponentially propagate them in the system until the local views converge. The second algorithm does not rely on global knowledge and adopts a heuristic method to achieve consensus on failures. The algorithms were implemented and tested using the Extreme-scale Simulator (xSim), ORNL’s performance/resilience investigation toolkit for simulating future-generation extreme-scale high-performance computing systems. The results show that in both algorithms the number of Gossip cycles to achieve global consensus scales logarithmically with system size. The second algorithm also shows better scalability in terms of memory usage and network bandwidth costs and a perfect synchronization in achieving global consensus.

This work was performed at the University of Reading, UK and ORNL. The work at ORNL was funded by DOE’s Advanced Scientific Computing Research office’s Exascale Operating System and Runtime (ExaOS/R) program.


Quantifying Scheduling Challenges for Exascale System Software

Oscar Mondragon, University of New Mexico, Patrick Bridges, University of New Mexico, Terry Jones, ORNL

The move towards high-performance computing (HPC) applications comprised of coupled codes and the need to dramatically reduce data movement is leading to a reexamination of time-sharing vs. space-sharing in HPC systems. In this paper, we discuss and begin to quantify the performance impact of a move away from strict space-sharing of nodes for HPC applications. Specifically, we examine the potential performance cost of time-sharing nodes between application components, we determine whether a simple coordinated scheduling mechanism can address these problems, and we research how suitable simple constraint-based optimization techniques are for solving scheduling challenges in this regime. Our results demonstrate that current general-purpose HPC system software scheduling and resource allocation systems are subject to significant performance deficiencies which we quantify for six representative applications. Based on these results, we discuss areas in which additional research is needed to meet the scheduling challenges of next-generation HPC systems.

This work is funded by DOE-ASCR and is part of the Hobbes project.

Science Highlights [Continued]

**Block Preconditioners for Implicit Atmospheric Climate Simulations**  
**P. A. Lott (LLNL), C.S. Woodward (LLNL), K.J. Evans (ORNL)**

In this paper, we introduce a scalable preconditioner within the Community Atmospheric Model (CAM) model that is designed to improve the efficiency of the linear system solves in the implicit dynamics solver. Performing accurate and efficient numerical simulation of global atmospheric climate models is challenging due to the disparate length and time scales over which physical processes interact. Implicit solvers enable the physical system to be integrated with a time step commensurate with processes being studied rather than to maintain stability. The dominant cost of an implicit time step is the ancillary linear system solves, so the preconditioner, which is based on an approximate block factorization of the linearized shallow-water equations, has been implemented within the spectral element dynamical core of CAM to minimize this expense. In this paper, we discuss the development and scalability of the preconditioner for a suite of test cases with the implicit shallow-water solver within CAM, and show how the choice of solver parameter settings affects the behavior of both the solver and preconditioner. We also present the remaining steps to gain efficiency using this solver strategy.  

This work is funded by DOE BER/ASCR and is part of the Multiscale BER SciDAC project  


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*# linear iterations with implicit solver with and without a preconditioner, using a 720s time step size, Williamson et al. 1992 test case; 1 day;*

**Table2Graph: A Scalable Graph Construction from Relational Tables using MapReduce framework**  
*Sangkeun Lee, Byung H. Park (Lead), Seung-Hwan Lim, and Mallikarjun Shankar*

Identifying correlations and relationships between entities within and across different data sets (or databases) is of great importance in many domains. The data warehouse-based integration, which has been most widely practiced, is found to be inadequate to achieve such a goal. Instead we explored an alternate solution that turns multiple disparate data sources into a single heterogeneous graph model so that matching between entities across different source data would be expedited by examining their linkages in the graph. We found, however, while a graph-based model provides outstanding capabilities for this purposes, construction of one such model from relational source databases were time consuming and primarily left to ad hoc proprietary scripts. This led us to develop a reconfigurable and reusable graph construction tool that is designed to work at scale.  

This work was sponsored by LDRD funds.  

Publication: Sangkeun Lee, Byung H. Park, Seung-Hwan Lim, and Mallikarjun Shankar, Table2Graph: A Scalable Graph Construction from Relational Tables using Map-Reduce, IEEE conference on BigData Services, 2015
Arguably one of the most important effects of climate change is the potential impact on human health. While this is likely to take many forms, the implications for future transmission of vector-borne diseases (VBDs), given their ongoing contribution to global disease burden, are both extremely important and highly uncertain. In part, this is owing not only to data limitations and methodological challenges when integrating climate-driven VBD models and climate change projections, but also, perhaps most crucially, to the multitude of epidemiological, ecological and socio-economic factors that drive VBD transmission.

This complexity has generated considerable debate over the past 10–15 years. In this review article, the authors seek to elucidate current knowledge around this topic, identify key themes and uncertainties, evaluate ongoing challenges and open research questions and, crucially, offer some solutions for the field. Although many of these challenges are ubiquitous across multiple VBDs, more specific issues also arise in different vector–pathogen systems.
Towards a Science of Tumor Forecast for Clinical Oncology
T. Yankeelov, V. Quaranta, K.J. Evans, and E. Rericha

We propose that the quantitative cancer biology community makes a concerted effort to apply lessons from weather forecasting to develop an analogous methodology for predicting and evaluating tumor growth and treatment response. Currently, the time course of tumor response is not predicted; instead, response is only assessed post hoc by physical examination or imaging methods. This fundamental practice within clinical oncology limits optimization of a treatment regimen for an individual patient, as well as to determine in real time whether the choice was in fact appropriate. This is especially frustrating at a time when a panoply of molecularly targeted therapies is available, and precision genetic or proteomic analyses of tumors are an established reality. By learning from the methods of weather and climate modeling, we submit that the forecasting power of biophysical and biomathematical modeling can be harnessed to hasten the arrival of a field of predictive oncology. With a successful methodology toward tumor forecasting, it should be possible to integrate large tumor-specific datasets of varied types and effectively defeat one cancer patient at a time.

This work was sponsored by DOE.


A Simple, Optical Method to Determine How Two-dimensional Layers are Stacked in a Crystal
Alexander A. Puretzky, Liangbo Liang, Xufan Li, Kai Xiao, Kai Wang, Masoud Mahjouri-Samani, Leonardo Basile, Juan Carlos Idrobo, Bobby G. Sumpter, Vincent Meunier, David B. Geohegan

In this work it was discovered that layers of two-dimensional (2D) materials with different atomic registries have characteristic Raman spectra fingerprints in the low frequency spectral range that can be used to characterize stacking patterns of these materials. Stacked monolayers of 2D materials present a new class of hybrid materials with tunable optoelectronic properties determined by their stacking orientation, order, and atomic registry. Fast optical determination of the exact atomic registration between different layers, in few-layer 2D stacks is a key factor for rapid development of these materials and their applications. Using two- and three-layer MoSe2 and WSe2 crystals synthesized by chemical vapor deposition we show that the generally unexplored low frequency Raman modes (< 50 cm⁻¹) that originate from interlayer vibrations can serve as fingerprints to characterize not only the number of layers, but also their stacking configurations. Ab initio calculations and group theory analysis corroborate the experimental assignments and show that the calculated low frequency mode fingerprints are related to the 2D crystal symmetries.

This work was sponsored by DOE.


Raman spectra of two-layer MoSe2 measured on a TEM grid for 2H and 3R stacking patterns verified by atomic resolution Scanning Transmission Electron Microscopy (STEM). Stokes (right) and anti-Stokes (left) terahertz Raman spectra of MoSe2 bilayers suspended on a TEM grid. The insets show atomic resolution STEM images of the 2H (top) and 3R (bottom) stacking patterns and their schematics taken at the locations used for the Raman measurements.
Web-based Visual Analytics for Extreme Scale Climate Science
C.A. Steed, K.J. Evans, J.F. Harney, B.C. Jewell, G. Shipman, B.E. Smith, P.E. Thornton, and D.N. Williams

In this paper, we introduce a Web-based visual analytics framework for democratizing advanced visualization and analysis capabilities pertinent to large-scale earth system simulations. We address significant limitations of present climate data analysis tools such as tightly coupled dependencies, inefficient data movements, complex user interfaces, and static visualizations. Our Web-based visual analytics framework removes critical barriers to the widespread accessibility and adoption of advanced scientific techniques. Using distributed connections to back-end diagnostics, we minimize data movements and leverage HPC platforms. We also mitigate system dependency issues by employing a RESTful interface. Our framework embraces the visual analytics paradigm via new visual navigation techniques for hierarchical parameter spaces, multi-scale representations, and interactive spatio-temporal data mining methods that retain details. Although generalizable to other science domains, the current work focuses on improving exploratory analysis of large-scale Community Land Model (CLM) and Community Atmosphere Model (CAM) simulations.

This work is funded by DOE-BER and is part of the ACME project.

Fast Fault Injection and Sensitivity Analysis for Collective Communications
Manjunath Gorentla Venkata, Kun Feng, Dong Li

The collective communication operations, which are widely used in parallel applications for global communication and synchronization, are critical for application’s performance and scalability. However, how faulty collective communications impact the application and how errors propagate between the application processes is largely unexplored. One of the critical reasons for this situation is the lack of fast evaluation method to investigate the impacts of faulty collective operations. The traditional random fault injection methods relying on a large amount of fault injection tests to ensure statistical significance require a significant amount of resources and time. These methods result in prohibitive evaluation cost when applied to the collectives.

In this work, we explore a novel tool named Fast Fault Injection and Sensitivity Analysis Tool (FastFIT) to conduct fast fault injection and characterize the application sensitivity to faulty collectives. The tool achieves fast exploration by reducing the exploration space and predicting the application sensitivity using Machine Learning (ML) techniques. A basis for these techniques is implicit correlations between MPI semantics, application context, critical application features, and application responses to faulty collective communications. The experimental results show that our approach reduces the fault injection points and tests by 97% for representative benchmarks (NAS Parallel Benchmarks (NPB)) and a realistic application (Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)) on a production supercomputer. Further, we explore statistically generalizing the application sensitivity to faulty collective communications for these workloads, and present correlation between application features and the sensitivity.

This work is funded by OLCF and is part of the FastFIT project.
Transfer of Lustre Expertise to the Community

Michael Brim, Jesse Hanley, Jason Hill, Neena Imam, Josh Lothian, Rick Mohr (UTK/NICS), Sarp Oral, Joel Reed, Jeffrey Rossiter

The Lustre 101 web-based course series is focused on administration and monitoring of large-scale deployments of the Lustre parallel file system. Course content is drawn from nearly a decade of experience in deploying and operating leadership-class Lustre file systems at the Oak Ridge Leadership Computing Facility (OLCF) at Oak Ridge National Laboratory (ORNL).

A primary concern in deploying a large system such as Lustre is building the operational experience and insight to triage and resolve intermittent service problems. Although there is no replacement for experience, it is also true that there is no adequate training material for becoming a Lustre administration expert. The overall goal of the Lustre 101 course series is to distill and disseminate to the Lustre community the working knowledge of ORNL administration and technical staff in the hope that others can avoid the trials and tribulations of large-scale Lustre administration and monitoring.

The Lustre Administration Essentials course is targeted at experienced system administrators who are relatively new to Lustre, but may have prior experience with other distributed and parallel file systems. Topics in this course include an introduction to Lustre, hardware selection and benchmarking strategies, Lustre software installation and basic configuration, Lustre tuning and LNet configuration, and basic file system administration and monitoring approaches.

This work was sponsored by DoD-HPC Research Program at ORNL
For more information please visit - http://lustre.ornl.gov/lustre101-courses/

System-Level Support for Composition of Applications

Brian Kocoloski, John Lange, Hasan Abbasi, David E. Bernholdt (ORNL PI), Terry R. Jones, Jay Dayal, Noah Evans, Michael Lang, Jay Lofstead, Kevin Pedretti, and Patrick G. Bridges

This paper presents a preliminary design study and initial evaluation of an operating system/runtime (OS/R) environment, Hobbes, with explicit support for composing HPC applications from multiple cooperating components. The design is based on our previously presented vision and makes systematic use of both virtualization and lightweight operating systems techniques to support multiple communicating application enclaves per node. In addition, it also includes efficient inter-enclave communication tools to enable application composition. Furthermore, we show that our Hobbes OS/R supports the composition of applications across multiple isolated enclaves with little to no performance overhead.

Work was performed at University of Pittsburgh, ORNL, Georgia Institute of Technology, Los Alamos National Laboratory, Sandia National Laboratories, and the University of New Mexico. Sponsored by the DOE, Office of Science, Advanced Scientific Computing Research (ASCR) program.

This work is funded by DOE-ASCR and is part of the Hobbes project.
Fidelity of Climate Extremes in High Resolution Global Climate Simulations

Michael Brim, Jesse Hanley, Jason Hill, Neena Imam, Josh Lothian, Rick Mohr (UTK/NICS), Sarp Oral, Joel Reed, Jeffrey Rossiter

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

This work is funded by DOE-BER and is part of the ACME project.

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

Microscopic Calculations Reveal a Surprising Conventional Nature of Exotic Pairing States

Y. Wang, T. Berlijn, P.J. Hirschfeld, D.J. Scalapino, T.A. Maier

Early calculations of the iron-based superconductors based on a spin fluctuation model of pairing had great success in predicting the superconducting ground state and the qualitative systematics of its variation with doping, etc. Recent proposals, however, have argued that these treatments have neglected the true symmetry of the crystalline layer containing Fe, which has pnictogen and chalcogen atoms in buckled positions, providing a strong potential on the electrons in the Fe plane and enforcing a unit cell with 2 Fe atoms. Several recent phenomenological treatments of the implications of this symmetry for pairing have argued that this aspect had been missed in the earlier 1-Fe unit cell calculations and that this potential can force a completely different electronic ground state, where so-called eta-pairing states with non-zero total momentum and exotic properties such as odd parity spin singlet symmetry and possible time reversal symmetry breaking contribute to the superconducting condensate. This work uses concrete and realistic microscopic calculations for 2-Fe and 1-Fe models to demonstrate that the earlier 1-Fe calculations correctly accounted for this glide-plane symmetry and correctly predicted its implications on the observable superconducting gap. It furthermore shows that eta-pairing naturally arises in systems where both orbitals with even and orbitals with odd mirror reflection symmetry in z contribute to the Fermi surface states. In contrast to the recent proposals, however, this study finds that eta-pairing contributes with the usual even parity symmetry and that time reversal symmetry is not broken. This work has established a clear framework for the study of such questions in other unconventional superconductors, where similar questions have also arisen.

This work is funded by DOE and NSF.

Science Highlights [Continued]

Wide-Area In Transit Data Processing For Real-Time Monitoring


ICEE addresses the challenges of building a remote data analysis framework, motivated from real-world scientific applications. ICEE is designed to support data stream processing for near real-time remote analysis over wide-area networks. This solution is based on in-memory stream data processing in which we can reduce the time-to-solution compared with conventional batch-based processing.

Work was performed by ORNL, LBNL, PPPL, Georgia Tech, Rutgers University, KISTI (Korea), A*STAR Computational Resource Centre (Singapore), and the ICEE SciDAC project for the wide-area-network movement.

Publications:
Publication: ICEE: Enabling data stream processing for remote data analysis over wide area networks. Special Issue in Supercomputing frontiers and innovations, 2015

Memory Scalability and Efficiency Analysis of Parallel Codes

Tomislav Janjusic and Christos Kartsaklis, ORNL

Memory scalability is an enduring problem and bottleneck that plagues many parallel codes. Parallel codes designed for High Performance Systems are typically designed over the span of several, and in some instances 10+, years. As a result, optimization practices, which were appropriate for earlier systems, may no longer be valid and thus require careful optimization consideration. Specifically, parallel codes whose memory footprint is a function of their scalability must be carefully considered for future exa-scale systems.

In this work we present a methodology and tool to study the memory scalability of parallel codes. Using our methodology we evaluate an application’s memory footprint as a function of scalability, which we coined memory efficiency, and describe our results. In particular, using our in-house tools we can pinpoint the specific application components, which contribute to the application’s overall memory foot-print (application data-structures, libraries, etc.).

This work was performed at ORNL using OLCF funding.

News

ACME continues to soar with yet another award
Launched in 2014, ACME is a multi-laboratory initiative to harness the power of supercomputers like ORNL’s Titan and Argonne’s Mira to develop fully coupled state-of-the-science Earth system models for climate change research and scientific and energy applications. Eight national labs, the National Center for Atmospheric Research, four academic institutions, and one private sector company are collaborating on the 10-year project. Researchers from ORNL’s Climate Change Science Institute (CCSI) were instrumental in developing and defending the project plan and are leading or co-leading several project teams, including the teams responsible for new land model development (Peter Thornton), assessing and improving model performance on high-performance computing platforms (Patrick Worley), and developing and evaluating simulation workflow tools (Kate Evans).
http://climatechangescience.ornl.gov/content/acme-continues-soar-yet-another-award

CSMD staff mentor HVA student
Harding Valley Academy’s Feldman ready to shed light on climate change
Following an internship at Oak Ridge National Laboratory (where he was mentored by CSMD’s Kate Evans), 18-year-old Sam Feldman not only has chosen his profession — he’s passionate about helping to reverse the effects of man-made climate change.

“That’s when I first found out about climate change research, and that got me interested,” Feldman, a Hardin Valley Academy 2015 graduate and advanced placement honors student, said. “All the data we studied pointed toward it being a reality. And the fact that ice sheets are melting [at the earth’s poles]. … I specifically studied ice sheets so I learned a lot about how they are currently melting.”
http://www.farragutpress.com/articles/2015/05/4006.html#sthash.p6PkJQ58.dYRQrzB.dpuf

Pavel Shamis (ORNL) and Gilad Shainer (Mellanox) announce the UCX Unified Communication X Framework.
UCX is a collaboration between industry, laboratories, and academia to create an open-source production grade communication framework for data centric and HPC applications
http://insidehpc.com/2015/05/slidecast-ucx-unified-communication-x-framework/

Jay Jay Billings Interview
CSMD researcher Jay Jay Billings was the subject of the latest User Spotlight interview which is part of the Eclipse Newsletter. The Eclipse technology is a vendor-neutral, open development platform supplying frameworks and exemplary, extensible tools (the “Eclipse Platform”).
To read the full interview please go here - To read the full interview please go here - https://www.eclipse.org/community/eclipse_newsletter/2015/july/?utm_source=twitterfeed&utm_medium=twitter&utm_campaign

Community Service

- Rick Archibald, Editor, International Journal of Computer Mathematics
- Rick Archibald, Committee member, Bredesen Center for Artem Maksov
- Rick Archibald, Committee member, SCALA14 committee (http://www.csm.ornl.gov/srt/conferences/Scala/2014/)
- Rick Archibald, IFIM technical lead for image analysis
- David E. Bernholdt chaired the panel on Software Integration and Performance at the 2015 DOE Workshop on Integrated Simulations for Magnetic Fusion Energy Sciences, 2-4 June 2015, Rockville, MD
- Wael ELwasif, Reviewer, papers for Euro-Par 2015 conference.
- Wael ELwasif, Reviewer, proposals for the Exascale initiative of the ORNL 2015 LDRD program.
- Christian Engelmann, Technical program committee member, 8th International Conference on Simulation Tools and Techniques (SIMUTools), Athens, Greece, August 24-25, 2015.

Community Service [Continued]


• Christian Engelmann, Peer reviewer, Journal of Parallel and Distributed Computing
• (JPDC), May, 2015.
• Christian Engelmann, Technical program committee member, 28th ACM/IEEE International Conference on High Performance Computing, Networking, Storage and Analysis (SC), Austin, TX, USA, November 15-20, 2015.
• Christian Engelmann, Technical program committee co-chair, 8th Workshop on Resiliency in High Performance Computing (Resilience) in Clusters, Clouds, and Grids, held in conjunction with the 21st International European Conference on Parallel and Distributed Computing (Euro-Par), Vienna, Austria, August 24-28, 2015.
• Christian Engelmann, Technical program committee member, 22nd European MPI Users’ Group Meeting (EuroMPI), Bordeaux, France, September 21-25, 2015.
• Kate Evans, Chair, Numerical and Computational Developments to Advance Multiscale Earth System Models (MSESM)
• Kate Evans, Organizer, CCSI Earth System Modeling Workshop
• Forrest Hoffman, Organizer, CCSI Earth System Modeling Workshop
• Forrest Hoffman, Chair, 6th Workshop on Data Mining in Earth System Science – DMESS
• Manjunath Gorentla Venkata, Program Committee Member, Advances in Computing, Communications and Informatics – Industry Track, ICACCI 2015
• Cory Hauck, Organizer, mini symposium - Computational Methods for Kinetic Equations and Related Models (5 parts), SIAM Conference on Computational Science and Engineering
• Cory Hauck, Organizer, mini symposium - Hybrid and Multilevel Approaches to Kinetic Equations (4 parts), SIAM Conference on Computational Science and Engineering
• Christos Kartsaklis, Program Committee Member, ICPP 2015:International Conference on Parallel Processing.
• Christos Kartsaklis, Program Committee Member, 17th IEEE International Conference on High Performance and Communications (HPCC 2015).
• Christos Kartsaklis, Program Committee Member, P2S2 2015: 8th International Workshop on Parallel Programming Models and Systems Software for High-End Computing.
• Christos Kartsaklis, Program Committee Member, ISPA 2015: The 13th IEEE International Symposium on Parallel and Distributed Processing with Applications.
• Christos Kartsaklis, Program Committee Member, 4th International Conference on Advances in Computing, Communications and Informatics (ICACCI).
• Christos Kartsaklis, Program Committee Member, 11th International Conference on Parallel Processing and Applied Mathematics (PPAM 2015).
• Christos Kartsaklis, Program Committee Member, 9th IEEE International Symposium on Embedded Multicore/Many-core Systems-on-Chip (MCSocC-15).
• Christos Kartsaklis, Program Committee Member, 3rd Workshop on Runtime and Operating Systems for the Many-core Era (ROME 2015), in conjunction with Euro-Par 2015.
• Christos Kartsaklis, Program Committee Member, Heterogeneous and Unconventional Cluster Architectures and Applications (HUCAA 2015), in conjuction with IEEE Cluster 2015.
• Christos Kartsaklis, Program Committee Member, CppCon: The C++ Conference 2015.
• Sarah Powers, Peer reviewed a book for IGI-Global.
• Pablo Seleson, Organizer, Computational and Applied Mathematics Seminar series at ORNL
• Pablo Seleson, Mentor, SULI students - Konrad Genser (University of Illinois at Urbana-Champaign) and Yohan John (Georgia Institute of Technology)
• Pablo Seleson, Reviewer, International Journal for Numerical Methods in Engineering
• Pablo Seleson, Reviewer, Mechanics Research Communications
• Pablo Seleson, Reviewer, SIAM Multiscale Modeling & Simulation
• Pavel Shamis, Chair, Interoperability Working Group Arbitration Committee for the Open Fabric Alliance (OFA).
• Pat Worley, Panelist, DOE Workshop on Integrated Simulations in Magnetic Fusion Energy Sciences
Events

**Second Software Expo in August!**
Jay Jay Billings

The second Oak Ridge National Laboratory Software Expo is planned for August 5 from 8:00 - 12:00 on Main Street and in the Court of Flags. Like last year, anyone is welcome to submit a project with all submissions guaranteed a spot! Only classified projects will not be accepted. Refreshments will once again be provided.

Last years expo was attended by over 170 people in addition to the 68 projects that were presented with projects ranging from internet technologies and business tools to scientific computing and parallel processing.

Detailed information about the expo is available at [http://www.csm.ornl.gov/expo](http://www.csm.ornl.gov/expo) and questions can be directed to ornl-software-expo@ornl.gov.

**ScalA’15: Workshop**
Christian Engelmann

ScalA’15: Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems. The 6th ScalA workshop will be held in conjunction with the International Conference on High Performance Computing, Networking, Storage and Analysis (SC) in Austin, TX on November 16. Papers are being accepted until August 14. For further details see [http://www.csm.ornl.gov/srt/conferences/Scala/2015](http://www.csm.ornl.gov/srt/conferences/Scala/2015) or contact the workshop program chair, Christian Engelmann at engelmannc@ornl.gov.

**WACCPD’15**
Oscar Hernandez

The 2nd Workshop on Accelerator Programming using Directives WACCPD’15 workshop will be co-located with SC15: International Conference on High Performance Computing, Networking, Storage and Analysis (SC) in Austin, TX on November 16. The call for papers is available at [http://www.openacc.org/content/events/WACCPD_2015](http://www.openacc.org/content/events/WACCPD_2015) and we are currently accepting papers until August 22nd, 2015. For more information about the workshop, please contact steering committee member Oscar Hernandez at oscar@ornl.gov.

**Towards Comprehensive System Comparison: Using the SPEC HPG Benchmarks for Better Analysis, Evaluation, and Procurement of next-generation HPC systems**
Oscar HernandezZ

Members SPEC High-Performance Group, including CSMD’s Oscar Hernandez, will be giving the tutorial 'Towards Comprehensive System Comparison: Using the SPEC HPG Benchmarks for Better Analysis, Evaluation, and Procurement of next-generation HPC systems' at SC’15. This tutorial will provide an overview of the SPEC HPG benchmark suites and focus in-depth on how to use the benchmarks and how to interpret the results. Participants will learn how to install, compile and run the benchmark and how to submit results to the SPEC website for publication. We show how to use the benchmarks to access compiler performance, tune system parameters, evaluate application scalability, compare systems, and monitor power consumption. For more information please contact Oscar Hernandez at oscar@ornl.gov

**ORNL OpenACC Meeting**

On May 12-14th, a three-day Face to Face OpenACC meeting took place at Oak Ridge National Laboratory to work towards the next versions of the OpenACC 2.5 specification. The OpenACC 2.5 is scheduled to be released on June 2015. The participants included the leading experts and researchers in the field of accelerator programming from PGI, NVIDIA, TU-Dresden, University of Houston, EPCC, TOTAL and ORNL.

On the first day, the committee met with scientific application developers from ORNL, critical codes that run as part of NCCS activities, including INCITE and CAAR. The codes include: ACME Land Model and ATM, One-Way Based Methods OWBM, Dalton, Maestro, LSMS-3, and Denovo/Sweep. These users are developers of some of the major scientific applications used on accelerator-based supercomputers such as Titan. They presented the results of their work with OpenACC but also explained their experiences and needs for the future.

For the following days, the OpenACC committee had technical discussions to integrate new features in OpenACC such as the new behavior for unstructured data constructs (reference counting), default behavior for data clauses, improved multi-accelerator API, a new OpenACC tools API, improved reduction operations for complex types, and improved asynchronous behavior for OpenACC APIs.

For more information please visit - [https://www.olcf.ornl.gov/training-event/openacc-f2f-2015/](https://www.olcf.ornl.gov/training-event/openacc-f2f-2015/)

**ESM Workshop**
Kate Evans and Forrest Hoffman

The Earth System Modeling (ESM) group conducted a day-long workshop covering global, coupled Earth system model (GCM) development and evaluation. The goals of the workshop were to educate participants about how GCM work and what the ESM group is doing to improve GCM to achieve DOE’s science goals. For more information please visit - [http://www.csm.ornl.gov/workshops/esm2015/index.html](http://www.csm.ornl.gov/workshops/esm2015/index.html)
Numerical and Computational Developments to Advance Multiscale Earth System Models (MSESM) Workshop
Kate Evans

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

CSMD Seminar Series
- June 30, 2015 - Torsten Hoefler: How fast will your application run at <next>-scale? Static and dynamic techniques for application performance modeling
- June 22, 2015 - Mohamed Wahib: Scalable and Automated GPU Kernel Transformations in Production Stencil Applications
- June 12, 2015 - Saurabh Hukerikar: Introspective Resilience for Exascale High Performance Computing Systems
- June 5, 2015 - Vivek Sarkar: Runtime System Challenges for Extreme Scale Systems
- May 27, 2015 - Jeffrey K. Hollingsworth: Active Harmony: Making Autotuning Easy
- May 19, 2015 - Mikolaj Fajer: Effects of the SH2/SH3 Regulatory Domains on the Activation Transition of c-Src Kinases
- May 14, 2015 - Brent Gorda: Lustre Keeping Pace with Compute and Intel’s Continued Commitment
- April 16, 2015 - David Lecomber: Software Engineering for HPC - Experiences in Developing Software Tools for Rapidly Moving Targets
- April 8, 2015 - Kirk W. Cameron: Why high-performance systems need a little bit of LUC

CAM Seminar Series
- April 2, 2015 - Analysis of Krylov Solver Resilience in the Presence of Soft-Faults, Dr. Miroslav Stoyanov, Oak Ridge National Laboratory
- April 9, 2015 - Non-local Models of Anomalous Transport, Dr. Diego Del-Castillo-Negrete, Oak Ridge National Laboratory
- April 16, 2015 - Structured and unstructured sampling methods for the approximation of parametric PDEs, Dr. Abdellah Chkifa, Oak Ridge National Laboratory
- April 23, 2015 - Coherent Lagrangian Vortices in Three-dimensional Unsteady Fluid Flows, Dr. Daniel Blazevski, Oak Ridge National Laboratory
- April 8, 2015 - Kirk W. Cameron: Why high-performance systems need a little bit of LUC
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Awards and Recognition
Pablo Seleson
Pablo Seleson was elected member of the United States Association for Computational Mechanics (USACM) Technical Thrust Area “Large Scale Structural Systems and Optimal Design” (http://www.usacm.org/technical_thrust_areas)

Tom Berlijn
Tom Berlijn’s paper "Interpretation of Scanning Tunneling Quasiparticle Interference and Impurity States in Cuprates" where the authors describe how they apply a recently developed method combining first principles based Wannier functions with solutions to the Bogoliubov–de Gennes equations to the problem of interpreting STM data in cuprate superconductors was highlighted on the cover of the journal Physical Review Letters. Publication: http://tinyurl.com/qdavk76
Publications of Note


Abstract: The recently synthesized freestanding four-atom-thick double-layer sheet of ZnSe holds great promise as an ultraflexible and transparent photoelectrode material for solar water splitting. In this work, we report theoretical studies on a novel three-atom-thick single layer sheet of ZnSe that demonstrates a strong quantum confinement effect by exhibiting a large enhancement of the band gap (2.0 eV) relative to the zinc blende (ZB) bulk phase. Theoretical optical absorbance shows that the largest absorption of this ultrathin single-layer sheet of ZnSe occurs at a wavelength similar to its four-atom-thick double-layer counterpart, suggesting a comparable behavior on incident photon-to-current conversion efficiency for solar water splitting, among a wealth of potential applications. The results presented herein for ZnSe may be generalized to other group II-VI analogues.


Abstract: The tunable optoelectronic properties of stacked two-dimensional (2D) crystal monolayers are determined by their stacking orientation, order, and atomic registry. Atomic-resolution Z-contrast scanning transmission electron microscopy (AR-Z-STEM) and electron energy loss spectroscopy (EELS) can be used to determine the exact atomic registration between different layers, in few-layer 2D stacks; however, fast optical characterization techniques are essential for rapid development of the field. Here, using two- and three-layer MoSe2 and WSe2 crystals synthesized by chemical vapor deposition, we show that the generally unexplored low frequency (LF) Raman modes (<50 cm−1) that originate from interlayer vibrations can serve as fingerprints to characterize not only the number of layers, but also their stacking configurations. Ab initio calculations and group theory analysis corroborate the experimental assignments determined by AR-Z-STEM and show that the calculated LF mode fingerprints are related to the 2D crystal symmetries.


Abstract: We apply a recently developed method combining first principles based Wannier functions with solutions to the Bogoliubov–de Gennes equations to the problem of interpreting STM data in cuprate superconductors. We show that the observed images of Zn on the surface of Bi2Sr2CaCu2O8 can only be understood by accounting for the tails of the Cu Wannier functions, which include significant weight on apical O sites in neighboring unit cells. This calculation thus puts earlier crude “filter” theories on a microscopic foundation and solves a long-standing puzzle. We then study quasiparticle interference phenomena induced by out-of-plane weak potential scatterers, and show how patterns long observed in cuprates can be understood in terms of the interference of Wannier functions above the surface. Our results show excellent agreement with experiment and enable a better understanding of novel phenomena in the cuprates via STM imaging.


Abstract: Graphitic carbon is still the most ubiquitously used anode material in Li-ion batteries. In spite of its ubiquity, there are few theoretical studies that fully capture the energetics and kinetics of Li in graphite and related nanostructures at experimentally relevant length, time-scales, and Li-ion concentrations. In this paper, we describe the development and application of a ReaxFF reactive force field to describe Li interactions in perfect and defective carbon-based materials using atomistic simulations. We develop force field parameters for Li–C systems using van der Waals-corrected density functional theory (DFT). Grand canonical Monte Carlo simulations of Li intercalation in perfect graphite with this new force field not only give a voltage profile in good agreement with known experimental and DFT results but also capture the in-plane Li ordering and interlayer separations for stage I and II compounds. In defective graphite, the ratio of Li/C (i.e., the capacitance increases and voltage shifts) both in proportion...
to the concentration of vacancy defects and metallic lithium is observed to explain the lithium plating seen in recent experiments. We also demonstrate the robustness of the force field by simulating model carbon nanostructures (i.e., both 0D and 1D structures) that can be potentially used as battery electrode materials. Whereas a 0D defective onion-like carbon facilitates fast charging/discharging rates by surface Li adsorption, a 1D defect-free carbon nanorod requires a critical density of Li for intercalation to occur at the edges. Our force field approach opens the opportunity for studying energetics and kinetics of perfect and defective Li/C structures containing thousands of atoms as a function of intercalation. This is a key step toward modeling of realistic carbon materials for energy applications.


Abstract: We present and demonstrate a novel protocol for distributing secret keys between two and only two parties based on N-party single-qubit Quantum Secret Sharing (QSS). We demonstrate our new protocol with N = 3 parties using phase-encoded photons. We show that any two out of N parties can build a secret key based on partial information from each other and with collaboration from the remaining N − 2 parties. Our implementation allows for an accessible transition between N-party QSS and arbitrary two party QKD without modification of hardware. In addition, our approach significantly reduces the number of resources such as single photon detectors, lasers and dark fiber connections needed to implement QKD. This work is supported by the U.S. Department of Energy under the Cybersecurity for Energy Delivery Systems (CEDS) program.


Abstract: A coherent array of regenerative amplifiers in an external cavity with a rank 1 scattering matrix is described and analyzed. Using a resonant cavity analysis, it is shown how the addition of regenerative feedback to each element in the array creates a phase shift relative to the well-known "cold-cavity phase shift." This phase shift is quantified and found to significantly affect the phasing properties of coherent arrays, even in the absence of the nonlinear Kerr effect and the gain-dependent phase shift. In particular, this regenerative phase shift is shown to concentrate the distribution of phases at the output of the laser array into a narrower phase range compared to the random distribution expected using a nonregenerative amplifier in the presence of effectively random cold-cavity phase shifts.


Abstract: We have coherently combined a high-power broad-area laser diode array by using a feedback loop closed off-axis external Talbot cavity. The off-axis feedback from two gratings provides transverse-mode control of broad-area lasers. The Talbot configuration of the external cavity implements diffractive coupling among laser diodes. Feedback from two gratings increases external cavity quality factor and spectrum selection capability. As a result, spatial coherence was improved and spectral linewidth was narrowed down. The high visibility of the far-field profile indicates that high spatial coherence was achieved. We also observed symmetric far-field profiles indicating that laser array was phase locked to in-phase and out-of-phase super-modes, respectively. Transition between these super-modes was observed by tuning one grating’s tilted angle. (C) 2010 Optical Society of America

B. Liu and Y. Braiman, “Coherent beam combining of high power broad-area laser diode array with near diffraction limited beam quality and high power conversion efficiency.” Optics Express 21(25), 31218-31228 (2013)

Abstract: We explored a path of achieving high quality phase-locking of broad-area laser diode (BALD) array that operates at high electrical to optical power conversion efficiency (PCE). We found that (a) improving single transverse mode control for each individual BALD, (b) employing global Talbot optical coupling among diodes, and (c) enhancing strength of optical coupling among diodes are key factors in achieving high quality phase-locking of high power BALD array. Subsequently, we redesigned and improved a V-shaped external Talbot cavity and employed low reflectivity anti-reflection (AR) coated, low-“smile” BALD array to meet these three important requirements. We demonstrated near-diffraction limit far-field coherent pattern with 19% PCE and 95% visibility. The far-field angle (full-width at half-maximum (FWHM)) of center lobe was measured as 1.5 diffraction angular limited with visibility of 99% for 5A injection current and 1.6 diffraction angular limited with visibility of 95% for 14A injection current. Power scaling of diode array is discussed. (C) 2013 Optical Society of America
Abstract: The physical layer describes how communication signals are encoded and transmitted across a channel. Physical security often requires either restricting access to the channel or performing periodic manual inspections. In this tutorial, we describe how the field of quantum communication offers new techniques for securing the physical layer. We describe the use of quantum seals as a unique way to test the integrity and authenticity of a communication channel and to provide security for the physical layer. We present the theoretical and physical underpinnings of quantum seals including the quantum optical encoding used at the transmitter and the test for non-locality used at the receiver. We describe how the envisioned quantum physical sublayer senses tampering and how coordination with higher protocol layers allows quantum seals to influence secure routing or tailor data management methods. We conclude by discussing challenges in the development of quantum seals, the overlap with existing quantum key distribution cryptographic services, and the relevance of a quantum physical sublayer to the future of communication security.

Link: http://ieeexplore.ieee.org/xpl/articleDetails.jsp?arnumber=6576339


Abstract: Adiabatic quantum programming defines the time-dependent mapping of a quantum algorithm into an underlying hardware or logical fabric. An essential step is embedding problem-specific information into the quantum logical fabric. We present algorithms for embedding arbitrary instances of the adiabatic quantum optimization algorithm into a square lattice of specialized unit cells. These methods extend with fabric growth while scaling linearly in time and quadratically in footprint. We also provide methods for handling hard faults in the logical fabric without invoking approximations to the original problem and illustrate their versatility through numerical studies of embeddability versus fault rates in square lattices of complete bipartite unit cells. The studies show that these algorithms are more resilient to faulty fabrics than naive embedding approaches, a feature which should prove useful in benchmarking the adiabatic quantum optimization algorithm on existing faulty hardware.


Abstract: The problem of detecting slowly-moving targets using airborne radars, particularly in the presence of background clutter and hostile electronic countermeasures or jamming, has led to the development of the space-time adaptive processing (STAP) algorithms in the radar community. However, the design of an optimal (or fully-adaptive) STAP-filter is computationally intensive and requires many homogeneous secondary-data which are often unavailable in practice. In this work, we employ an orthogonal frequency division multiplexing (OFDM) radar to detect a target using a sparsity-based STAP technique. We observe that the target and interference spectra are inherently sparse in the spatio-temporal domain. Hence, we exploit that sparsity to develop an efficient STAP technique that utilizes considerably lesser number of secondary data and produces an equivalent performance as the other existing STAP techniques. In addition, the use of an OFDM signal increases the frequency diversity of our system as the OFDM-STAP filter-weights can be made adaptable to the frequency-variations of the target and interference responses. Hence, by better utilizing the frequency variabilities, we adaptively design the OFDM waveforms, and consequently gain a significant amount of STAP-performance improvement.


Abstract: The problem of detecting slowly-moving targets in urban environments, for example in an urban environment, is becoming increasingly relevant and challenging to radar technologies. Along with the multipath reflections, an urban canyon is full of refractions and scattering from different structures around the target, and often the line-of-sight (LOS) propagation path from the radar to the target is not available. Therefore, solving this problem requires the exploitation of multipath reflections rather than canceling them. In this work, we take advantage of the multipath propagation that increases the spatial diversity of the radar system and provides multiple Doppler shifts corresponding to the projections of the target velocity on each of the multipath components. To resolve and exploit the multipath components, we use a wideband OFDM signaling scheme. We develop a parametric measurement model under the generalized multivariate analysis of variance (GMANOVA) framework, and employ the generalized likelihood ratio (GLR) tests to decide about the presence of a target in a particular range cell. Then, we evaluate the asymptotic performance analysis of the
Publications of Note [Continued]

detector, and propose an algorithm to optimally design the parameters of the OFDM transmitting waveform for the next coherent processing interval. Our numerical examples illustrate the performance characteristics of the proposed detector, and demonstrate the achieved performance improvement due to adaptive OFDM waveform design.


Abstract. UltraScience Net is a network research testbed for supporting the development and testing of wide-area networking technologies for high-performance computing and storage systems to support large-science applications. It provides dynamic, dedicated, high-bandwidth channels to support large data transfers, and also provides stable high-precision channels to support fine command and control operations. Its data-plane consists of 8,600 miles of cross-country dual OC192 backbone, which can be dynamically provisioned at different bandwidths. Its out-of-band control-plane is implemented using hardware Virtual Private Network (VPN) devices. In terms of the testbed infrastructure, it demonstrated the following capabilities: (i) ability to build and operate national-scale switched network testbeds, (ii) provisioning of suites of 1 and 10 Gbps connections of various lengths up to 70,000 and 8,600 miles, respectively, through automated scripts, (iii) secure control-plane for signaling and management operations, and (iv) bandwidth scheduler for in-advance connection reservation and provisioning. A number of structured and systematic experiments were conducted on this facility for the following tasks: (i) performance analysis and peering of layer 1-3 connections and their hybrid concatenations, (ii) scalability analysis of 8Gbps InfiniBand (IB) transport over wide-area connections of thousands of miles, (iii) diagnosis of TCP performance problems in using dedicated connections to supercomputers, (iv) detailed TCP performance analysis of wide-area application acceleration devices, and (v) TCP throughput improvements due to 10Gbps High Assurance Internet Protocol Encryptor (HAIPE) devices.


Abstract: The operation of cyber infrastructures relies on both cyber and physical components, which are subject to incidental and intentional degradations of different kinds. Within the context of network and computing infrastructures, we study the strategic interactions between an attacker and a defender using game-theoretic models that take into account both cyber and physical components. The attacker and defender optimize their individual utilities, expressed as sums of cost and system terms. First, we consider a Boolean attack-defense model, wherein the cyber and physical subinfrastructures may be attacked and reinforced as individual units. Second, we consider a component attack-defense model wherein their components may be attacked and defended, and the infrastructure requires minimum numbers of both to function. We show that the Nash equilibrium under uniform costs in both cases is computable in polynomial time, and it provides high-level deterministic conditions for the infrastructure survival. When probabilities of successful attack and defense, and of incidental failures, are incorporated into the models, the results favor the attacker but otherwise remain qualitatively similar. This approach has been motivated and validated by our experiences with UltraScience Net infrastructure, which was built to support high-performance network experiments. The analytical results, however, are more general, and we apply them to simplified models of cloud and high-performance computing infrastructures.
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

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