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QUARTERLY NEWSLETTER FOR
THE COMPUTER SCIENCE AND
MATHEMATICS DIVISION

CSMD

this issue

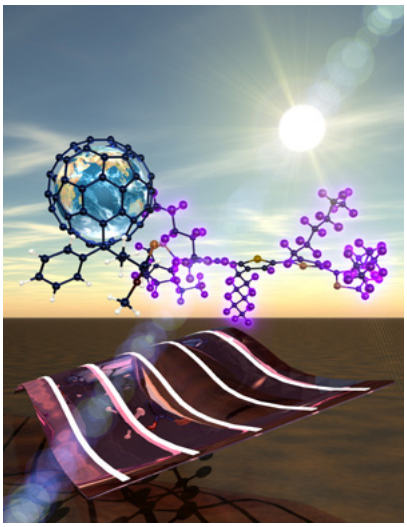
Science Highlights

Multidisciplinary ORNL team discovers unexpected effect of heavy hydrogen in organic solar cells

Photovoltaic spray paint could coat the windows and walls of the future if scientists are successful in developing low-cost, flexible solar cells based on organic polymers. Scientists at the Department of Energy's Oak Ridge National Laboratory recently discovered an unanticipated factor in the performance of polymer-based solar devices that gives new insight on how these materials form and function.

"One of the dreams is to bring home some polymer paint from the hardware store, spray it on a window and make your own solar cell because it self-orders into a structure that can generate electricity," ORNL's David Geohegan said. "But right now there are many unknown things that happen when you spray it down and it dries. Changing the electrical property of a polymer also changes its structure when it dries, so understanding this process is one of our big science mysteries."

When ORNL scientists Kai Xiao and Kunlun Hong analyzed neutron scattering data obtained at the lab's Spallation Neutron Source to measure the structure of seemingly identical polymer-based solar devices, they stumbled upon a new piece to the scientific solar puzzle.



Conceptual drawing shows a flexible organic photovoltaic made from an acceptor of PCBM (buckyball with earth) and the donor of deuterated conducting polymer. The polymer blend in the device (bottom) will harvest the sunlight to generate electrical power. (carbon:blue; sulfur: yellow; hydrogen: white; deuterium: purple). Image by Christopher Rouleau at ORNL's CNMS.

Read the rest of the story [**here**].

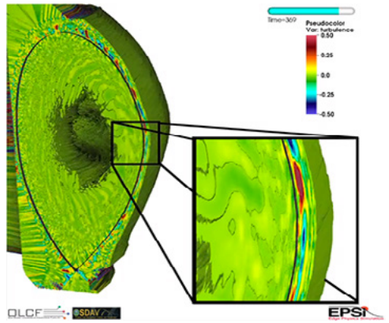
OAK RIDGE National Laboratory

Science Highlights [Continued]

CSMD Researchers Speed Along Fusion Research

ORNL Team Members: Ed D'Azevedo, Pat Worley, and Dave Pugmire

CSMD researchers Ed D'Azevedo and Pat Worley were part of a team led by Princeton Plasma Physics Laboratory's C.S. Chang. The team increased the performance of its fusion XGC1 code fourfold on ORNL's Titan supercocmputer using Titan's GPUs and CPUs, compared to its previous CPU-only incarnation after a 6-month performance engineering period.



This visualization shows the turbulence front from the plasma edge being spread inward in multiscale interaction with the evolving background profile under the central heat source. Eventually, the whole volume becomes turbulent, with the spatial turbulence amplitude distribution being just enough to produce the outward heat transport to expel the centrally deposited heat to the edge. The edge turbulence source is continuously fed by the heat flux from the core. This is how the plasma profile, the heat source and the turbulence self-organize.
Credit: Dave Pugmire, ORNL.

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

Publication in March 2014 Cluster Computing

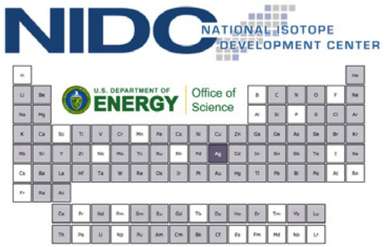
ORNL Team Members: Terry Jones and Stephen Poole

Computer Science Research Group member Terry Jones co-authored a paper describing recent successes from a collaboration between ORNL, the IOFSL Project, and the Vampir Project. The paper describes how the collaboration successfully improved the scaling capabilities of programming development tools. Programming development tools are a vital component for understanding the behavior of parallel applications. Event tracing is a principal ingredient to these tools, but new and serious challenges place event tracing at risk on extreme-scale machines. As the quantity of captured events increases with concurrency, the additional data can overload the parallel file system and perturb the application being observed. In this work, the authors presented a solution for event tracing on extreme-scale machines by increasing the maximum traced application size by a factor of 5x to more than 200,000 processes.

Thomas Ilsche, Joseph Schuchart, Joseph Cope, Dries Kimpe, Terry Jones, Andreas Knuepfer, Kamil Iskra, Robert Ross, Wolfgang E. Nagel, and Stephen W. Poole. **Optimizing I/O Forwarding Techniques for Extreme-Scale Event Tracing. Cluster Computing. March 2014, Volume 17, Issue 1, pp 1-18. doi:10.1007/s10586-013-0272-9**.

IBOBSU Website Enhancements: Progress Update

ORNL Team Members: Eric Lingerfelt, Michael Smith, Mitch Ferren, Monty Middlebrook



The National Isotope Development Center (NIDC) is the sole government source of stable and radio-isotope products for science, medicine, security, and applications. The NIDC manages the sales and distribution of these isotopes through the Isotope Business Office (IBO), which is located at ORNL. The Isotope Business Office Business Systems Upgrade (IBOBSU) project is an 18-month project begun in Summer 2013 that is focused on two separate tasks. The first task involves integrating the IBO's two internal business systems while the second task is comprised of major enhancements to the NIDC website at isotopes.gov and the NIDC Online Management Toolkit (OMT). Multiple milestones associated with the second task have been successfully achieved in the last three quarters. Website enhancements associated with these milestones include an online application for preferred customer status, a secure online quotation and ordering capability of stable isotopes from inventory for preferred customers, an online shopping cart feature for quote requests, and an online tool for preferred customer profile management. In addition to these deliverables, the 1.2 and 1.3 releases of the OMT provide software tools for NIDC staff that allow them to manage preferred customer accounts and process orders placed through the website.

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

Awards and Recognition

Postdoctoral Researcher Tianyu Jiang Awarded in "Best Dissertation" Competition

Tianyu Jiang, a postdoctoral researcher at Oak Ridge National Laboratory's Climate Change Science Institute, achieved 3rd place in the Chinese-American Oceanic and Atmospheric Association's "best dissertation" competition. Jiang, a member of CCSI's Earth System Modeling Group, received the award February 5 in Atlanta during the 94th annual meeting of the American Meteorological Society.

Jiang said what gave him the upper hand in the competition was a summer spent as a part of ORNL's Higher Education Research Experiences program, under the supervision of Kate Evans, leader of the ORNL Computational Earth Sciences Group and a member of CCSI. "My experience here was world class," said Jiang. "I had the chance to use high-performance computers and collaborate with the entire team to do cutting-edge work."

Jiang's thesis, "Understanding the Scale Interaction of Atmospheric Transient Disturbances and Its Coupling with the Hydrological Cycle over the Pacific-North American Regions," focused on the connection between climate over the North Pacific and extreme weather—freezing temperatures, high-impact precipitation, droughts, and other severe events. "Understanding extreme weather under a changing climate is becoming more and more challenging and urgent, not only because of the public's immediate need for weather information, but also the increasing concern from policymakers," said Jiang.—by Justin Kaffka

Paul Kent was elected as a member at large in the American Physical Society, Division of Computational Physics (DCOMP).

Forrest Hoffman's paper "Causes and Implications of Persistent Atmospheric Carbon Dioxide Biases in Earth System Models" was recognized as the most downloaded paper from the Journal of Geophysical Research: Biogeosciences for the month of February. The complete author's list and information can be found [**here**].

Roisin Langan was accepted to the University of Tennessee's Center for Interdisciplinary Research and Graduate Education (CIRE) PhD program and will be working with Kate Evans on the PISCEES project to verify and validate continental scale ice sheet models.

Clayton Webster was elected Frontier of Science Fellow for the National Academy of Sciences.

A committee of National Academy members selects the Fellows from among the best young scientists in a broad range of science disciplines. Clayton was selected for his work in uncertainty quantification and he presented an overview of the field at the Kavli Frontiers of Science symposium, jointly organized by the Humboldt Foundation and the US National Academy of Sciences, April 4-7, 2014.

Staff

Kate Evans, Computational Earth Sciences Group

The Computer Science and Mathematics Division (CSMD) is pleased to announce the appointment of Dr. Kate Evans as the Group Leader for the Computational Earth Sciences Group within CSMD, effective January 1, 2014. Kate has been the interim group leader since February 2013, succeeding Danny McKenna, who has moved to the Graduate Education and University Partnership Division. Kate received her Ph.D. from Georgia Institute of Technology in Atmospheric Science and her B.S. from Haverford College in Physics. Kate will be responsible for leading and continuing to develop a top notch research capability in computational Earth science.

Bobby Sumpter, Deputy Director of the Center for Nanophase Materials Sciences

Bobby G. Sumpter has accepted the position as Deputy Director of the Center for Nanophase Materials Sciences (CNMS).

Bobby received his Ph.D. in Physical Chemistry from Oklahoma State University in 1986. Following postdoctoral studies in Chemical Physics at Cornell University and in Polymer Chemistry at the University of Tennessee, Bobby joined the Chemistry Division at Oak Ridge National Laboratory as a staff member in the Polymer Science group. Bobby's research is focused on the fundamental understanding of self-assembly processes, interactions at interfaces, the structure and dynamics of molecular-based

Staff [Continued]

materials, and the physical, mechanical and electronic properties of nanoscale materials. His research uses a broad spectrum of materials theory and large-scale simulation approaches, including electronic structure and molecular dynamics. Working at the confluence of theory and experiment, he has authored over 300 scientific publications and several patents. He was named Corporate Fellow in 2013.

Bobby has been a staff member of the Center for Nanophase Materials Sciences since 2007 and the group leader for the Nanomaterials Theory Institute (NTI) at the CNMS since 2009. He is also the group leader of the Computational Chemical and Materials Sciences (CCMS) group in the Computer Science and Mathematics Division. Bobby will continue to serve as acting group leader for both the NTI and CCMS.

Clayton Webster,
Computational and Applied Mathematics Group

The Computer Science and Mathematics Division (CSMD) is pleased to announce the appointment of Dr. Clayton Webster as the Group Leader for the Computational and Applied Mathematics Group within CSMD. Clayton received his Ph.D. from Florida State University in Applied and Computational Mathematics and his M.S. from McMaster University in Applied Mathematics.

Clayton will be responsible for leading and continuing the development of research capability in mathematics.

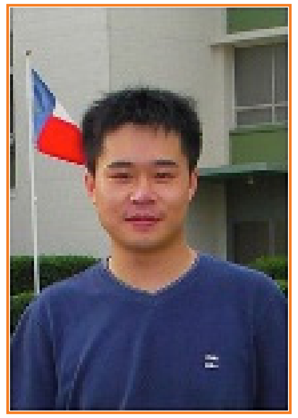
Jyoti P (JP) Mahalik,
Computational Chemical and Materials Sciences Group

JP Mahalik is a new postdoctoral researcher in CCMS Group. JP will be working on the field theory of polymer brushes. He is also developing a code for numerically computing the density profile of the polymer brushes and compare the results with the neutron reflectivity data.

Sophie Blondel,
Computer Science Research Group

Sophie Blondel started her postdoctoral appointment in the Computer Science Research group in January. She received her Ph.D. in physics from Paris-Sud University (France) in 2013, after working on the NEMO experiment and focusing specifically on particle detectors for double-beta decay measurements, by developing software to analyze eight years of data. Her current position on the Xolotl Plasma Surface Interaction project in Jay Billings's team is a good opportunity to improve her programming skills while utilizing her physics background, by working on uncertainty quantification and the visualization of Xolotl-PSI outputs.

Wei Ding
Computer Science Research Group



Wei Ding is a post-doctoral researcher in the Computer Science Research Group. He earned his Ph.D. in Computer Science from the University of Houston in 2013. Wei's research background is high-performance computing, heterogeneous computing, compiler optimization and performance analysis tool development. He is the main developer of the "Klonos", a tool that is used for scientific application porting based on code similarity analysis. Currently, he is working on a LDRD project for the OpenACC language extension and compiler development for porting applications to GPUs.

Community Service

- Rick Archibald, Member, ORNL Operations Committee
- Rick Archibald, Editor, International Journal of Computer Mathematics
- Rick Archibald, Organizer, SIAM UQ workshop: Efficient Simulation of Rare Event
- Rick Archibald, Member, Thesis advisory committee for Gabriel Wasserman, ASU
- David E. Bernholdt, program committee, 14th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid)

Community Service [Continued]

- David E. Bernholdt, organizing committee, ASCR Workshop on Software Productivity for Extreme-Scale Science (SWP4XS)
- David E. Bernholdt, reviewer, Computing in Science and Engineering
- David E. Bernholdt, invited participant, BER Workshop on Computational Challenges for Mechanistic Modeling of Terrestrial Environments (CCMMTE)
- David E. Bernholdt, PhD thesis external examiner, Australian National University
- Ed d'Azevedo, Co-organizer, Mini symposium "Solving Large-scale Linear Systems of Equations on Heterogeneous Distributed-memory Computers" at the SIAM Conference on Parallel Processing for Scientific Computing (PP14) Feb 18-21, 2014
- Ed d'Azevedo, Co-organizer, Mini symposium "Recent Advances in Particle-in-Cell Method on Multicore and GPU Systems" at the SIAM Conference on Parallel Processing for Scientific Computing (PP14) Feb 18-21, 2014
- Eirik Endeve, Reviewer, Article for Classical and Quantum Gravity
- Christian Engelmann, technical program committee vice-chair (programming models, systems and fault-tolerant computing track), IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid) 2014
- Christian Engelmann, reviewer, IEEE Transactions on Computers (TC)
- Christian Engelmann, technical program committee member, Workshop on Solving Problems with Uncertainties, in conjunction with the International Conference on Computational Science (ICCS) 2014
- Igor Jouline was elected as the vice-chair (in 2016) and chair (in 2018) of the Gordon Research Conference on Sensory Transduction in Microorganisms
- Christos Kartsaklis, Program Committee Member, The 24th ACM Workshop on Network and Operating Systems Support for Digital Audio and Video (NOSSDAV) co-located with ACM Multimedia Systems 2014 (MMSys 2014)
- Christos Kartsaklis, Program Committee Member, Tools for Program Development and Analysis in Computational Science workshop at the International Conference on Computational Science 2014 (ICCS 2014)
- Christos Kartsaklis, program committee member, 19th International Workshop on High-Level Parallel Programming Models and Supportive Environments (HIPS 2014), in conjunction with the 28th IEEE International Parallel & Distributed Processing Symposium (IPDPS 2014)
- Seyong Lee, Reviewer, ACM Transactions on Architecture and Code Optimization (TACO), 2014
- Dong Li, program committee, IEEE/ACM CCGrid 2014
- Dong Li, program committee, The Fourth International Workshop on Accelerators and Hybrid Exascale Systems, in association with IEEE International Parallel and Distributed Processing Symposium, 2014
- Dong Li, program committee, International Supercomputing Conference, 2014
- Dong Li, Program Committee, poster session, International Conference on Performance Engineering, 2014
- Tiffany M. Mintz, judge, Tennessee Technology Student Association (TSA) State Conference Inventions & Innovations event
- Sarah Powers, FY14 Householder selection committee member, ORNL
- Sarah Powers, technical reviewer, RNSD Level-3 milestone report, ORNL
- Pavel Shamis, co-chair, First OpenSHMEM Workshop: Experiences, Implementations and Tools
- Sarat Sreepathi, Reviewer, DOE Small Business Innovation Research (SBIR) Phase II proposals, 2014
- Miroslav Stoyanov, Contributor, Science Saturday at West High School
- John Turner, External Reviewer, Los Alamos National Laboratory LDRD titled "Disruptive Innovation in Numerical Hydrodynamics"
- Geoffroy Vallee, program committee, 5th International Conference on Cloud Computing, GRIDs, and Virtualization
- Jeffrey Vetter, Program Committee, ACM ICS 2014
- Jeffrey Vetter, Program Committee, ACM PPOPP 2014
- Jeffrey Vetter, Technical Program Deputy Chair, SC14
- Clayton Webster, Member, ORNL Seed Committee
- Clayton Webster, Member, ORNL Russell Fellowship Committee
- Clayton Webster, Chair, ORNL Householder Fellowship
- Clayton Webster, Member, Organizing Committee: SIAM Meeting on Uncertainty Quantification, March 31 - April 4
- Clayton Webster, Organizer, SIAM UQ mini-symposium: Numerical Approximation of High-dimensional Stochastic Equations (4 parts)
- Clayton Webster, Organizer, SIAM UQ mini-symposium: Uncertainty Quantification Driven by Large-Scale Applications
- Clayton Webster, Organizer, SIAM UQ mini-symposium: Uncertainty in Environmental Evaluation and Management (2 parts)
- Clayton Webster, Organizer, SIAM UQ mini-symposium: Uncertainty Quantification for Extreme-scale High Performance Computing

Community Service [Continued]

- Clayton Webster, Chair, SIAM UQ: The Theory Behind Reduced Basis Methods
- Patrick Worley, Program Committee, LSPP 2014
- Patrick Worley, Associate Editor, Parallel Computing

Conference on Data Analysis (CoDA) 2014

CSMD had a strong presence at the CoDA conference, which is a new biennial conference series for "Exploring Data-Focused Research Across the Department of Energy" that takes place in Santa Fe, NM. This year's conference was March 5-7. The invited program featured sessions on data-intensive applied science, uncertainty quantification, national security, big data and exascale computing, energy and the environment, and signature discovery. ORNL participation included all aspects of the conference:

- George Ostrouchov (CSMD/SDG), Organizing Committee and Poster
- Kate Evans (CSMD/CES), Plenary talk
- Yuan Tian (CSMD/SDG), Invited talk
- Cynthia Gu (CSMD/SDG), Poster
- Damian M. Maddalena (CSMD/CES), Poster
- Sarah Powers (CSMD/CSR), Poster

The conference had a single track of plenary and invited talks and a poster session. Many have noted that this was likely the best conference of the year due to its great opportunities for interaction between attendees. On the fun side, the conference banquet talk was by Amanda Cox, a Graphics Editor at the New York Times, who recently won the American Statistical Association's Excellence in Statistical Reporting Award. Her talk was on "Sketching the News: Data Graphics at the New York Times." As a side note, the 2012 conference banquet talk was "Blowing Stuff Up for Science: Explosives Experiments with the Myth Busters." These will be hard to surpass at the next meeting in 2016.

Eclipse Foundation

Jay Jay Billings

ORNL joined the Eclipse Foundation, which manages both an open source community and the development of the popular Eclipse Integrated Development Environment. The effort to join the Foundation was led by Jay Jay Billings of the Computer Science Research group to address several pressing issues for the NEAMS Integrated Computational Environment (NiCE).

Membership in the Foundation includes many benefits and applies site-wide to all UT-Battelle employees and subcontractors (including ORAU/ORISE post-graduates). In addition to providing access to a user base of more than nine million users for Eclipse projects, the Eclipse Foundation also provides marketing and advertising support, intellectual property-friendly contributor agreements to help with contributions to projects from third-party developers and access to hundreds of skilled developers from some of the biggest (and smallest!) companies in the tech sector. The process of proposing new projects is also streamlined for members since the necessary agreements are already in place.

Membership also allows ORNL to participate in the new Eclipse Science Working Group (SWG). The SWG is focused on creating new, science-focused Eclipse projects with completely new code bases or contributions from Foundation members in a technology-agnostic setting (read "not only Java projects"). The SWG also acts as a support community related to scientific activities projects with Eclipse.

Jay pursued membership in the Foundation primarily because of growing contributions from external collaborators to NiCE. Each contributing organization has its own set of policies related to open source software, intellectual property rights and code contributions, so the easiest and safest route was to creating a new project with a third party software Foundation. Since NiCE is based on the Eclipse Rich Client Platform and the NiCE team has been involved with the community for a number of years, the Eclipse Foundation was the obvious choice. A proposal to create the Eclipse Integrated Computational Environment, with NiCE as the initial contribution, is currently under review.

Software

DOE Accelerated Climate Modeling for Energy Workflow

Benjamin Mayer[1], Renata McCoy[2], Rachana Ananthakrishnan[3], Eric Blau[3], Zoe Guillen[4], Carla Hardy[2], Matthew Harris[2], Lukasz Lacinski[3], Carina Lansing[4], Elo Leung[2], Marcia Branstetter[1], John Harney[1], Brian Jewel[1], John Quigley[1], Brian Smith[1], Chad Steed[1], Kerstin Kleese-Van Dam[4], Kate Evans[1], Galen Shipman[1], Dean Williams[2]

1: Oak Ridge National Lab 2: Lawrence Livermore National Laboratory 3: Argonne National Lab 4: Pacific Northwest National Laboratory

The DOE BER is consolidating many projects with the Earth System Modeling program to create a high resolution coupled climate model capability. The workflow component of this has the goal of increasing the rate of scientific discovery by reducing the effort needed to set and run experiments, enable more complex representations of the Earth system at multiple and interacting scales to be included per computation allocation, and providing reproducibility of experiments. To accomplish this, we are building an automated workflow that builds a model configuration across all components and coordinates it execution on LCF systems such as OLCFs Titan and ALCF's Mira and handles all of the data transfer, publication, diagnostics, and provenance.

Software [Continued]

QITKAT

ORNL Team Member: Travis Humble

CSMD has recently upgraded the Quantum Information Tool Kit for Application Testing (QITKAT) library to implement new protocols for quantum communication. QITKAT is a software-defined communication architecture that uses real-time, stream-based processing to implement novel approaches to communication using quantum physics. Recent updates include the incorporation of error corrected dense coding as well as entanglement detection modules. QITKAT is currently being used to drive several quantum optics experiments at ORNL and the software has recently been picked up by the Army Research Laboratory for the development of software-defined quantum network protocols. Technical details are available in T. S. Humble and R. J. Sadlier, "Software-defined Quantum Communication Systems[2] (preprint, arXiv:1403.3270 [quant-ph])

Cheetah Framework for Collective Operations, Version 1.5

ORNL Team Member: Manju Gorentla Venkata

Cheetah is a framework for implementing blocking and nonblocking collective operations. It enables building high-performing collective operations by taking advantage of communication hierarchies in the multi-core systems, tailoring algorithms and implementations to specific communication hardware characteristics, and enabling computation-communication overlap.

Cheetah 1.5, the second version, can be downloaded as a part of Open MPI developers trunk, a popular implementation of MPI-2 standard; this version of Cheetah will also be part of Open MPI 1.7.5 series. This revision includes scalable implementation of Allreduce, Reduce, and Allgather collective operations. The performance analysis of these collectives on various architectures has been published in this paper: "Optimizing blocking and nonblocking reduction operations for multicore systems: Hierarchical design and implementation", Cluster 2013. This version is a joint effort of Oak Ridge National Laboratory and Los Alamos National Laboratory.

The first version of Cheetah was released in 2012, and it included the infrastructure to implement collectives, and a reference implementation of Barrier and Broadcast collective operations. The reference implementation outperforms the native implementations on Cray XE/XK and InfiniBand systems, and scales to over 100 thousand cores on Cray XE/XK systems. The scalability and performance results of Cheetah on various architectures are published in over 12 peer-reviewed conference and workshop publications.

Contact: Manju Gorentla Venkata, manjugv@ornl.gov
URL: **http://www.csm.ornl.gov/cheetah/**

National Isotope Development Center (NIDC) Online Management Toolkit (OMT) 1.3

ORNL Team Member: Eric Lingerfelt

The National Isotope Development Center (NIDC) Online Management Toolkit (OMT) provides NIDC staff the capability to quickly and securely modify the product catalog, harvest website statistics, dynamically generate monthly reports, administer OMT user accounts, and manage NIDC Preferred Customer account with a web-deliverable, cross-platform Java application. A major milestone in the Isotope Business Office Business Systems Upgrade (IBOBSU) project has been achieved with the release of OMT 1.3. A central goal of IBOBSU is to create a NIDC Preferred Customer Portal at isotopes.gov that allows vetted research customers the ability to create quotes and submit orders for stable isotopes in inventory via the website. The latest OMT tool, called the "Online Order Manager", allows NIDC staff to explore, process, and delete online orders submitted through isotopes.gov. The tool also allows staff to export online orders as an Excel spreadsheet and as a fillable PDF of DOE Isotope and Technical Service Order Form CA-10-90.COM Rev 3.

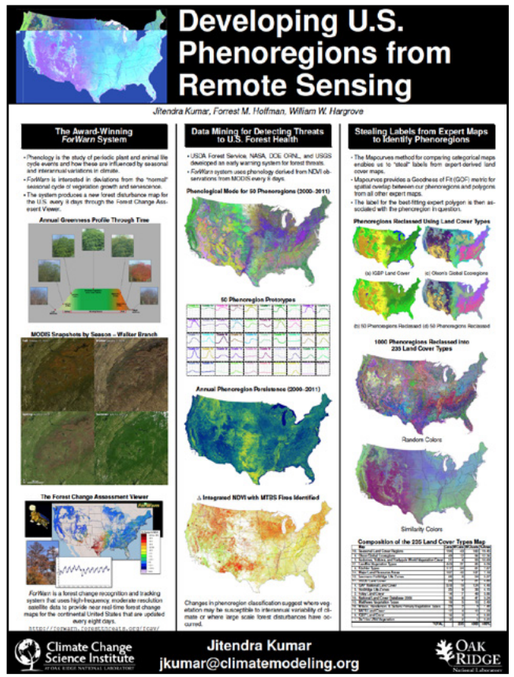
Contact: Eric Lingerfelt, lingerfeltej@ornl.gov
URL: **isotopes.gov**

Events

Advisory Council Review

The third annual meeting of the Oak Ridge National Laboratory Computing and Computational Sciences Directorate (CCSD) advisory committee was convened March 6-7 to focus on two key areas of Directorate activities. The primary activities were to review CCSD's recent developments in computational and applied mathematics and CCSD's geospatial data science program and its impact on problems of national and global significance.

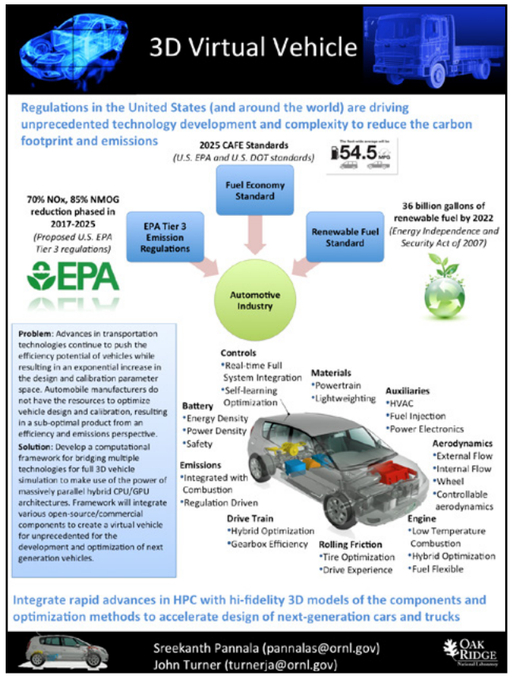
In the course of the review, CSMD researchers presented five posters covering their work in computational and applied mathematics.



Developing U.S. Phenoregions from Remote Sensing

Jitendra Kumar, Forrest Hoffman, and William Hargrove

Variations in vegetation phenology can be a strong indicator of ecological change or disturbance. Phenology is also strongly influenced by seasonal, interannual, and long-term trends in climate, making identification of changes in forest ecosystems a challenge. Normalized difference vegetation index (NDVI), a remotely sensed measure of greenness, provides a proxy for phenology. NDVI for the conterminous United States (CONUS) derived from the Moderate Resolution Spectroradiometer (MODIS) at 250 m resolution was used in this study to develop phenological signatures of ecological regimes called phenoregions. By applying a unsupervised, quantitative data mining technique to NDVI measurements for every eight days over the entire MODIS record, annual maps of phenoregions were developed. This technique produces a prescribed number of prototypical phenological states to which every location belongs in any year. Since the data mining technique is unsupervised, individual phenoregions are not identified with an ecologically understandable label. Therefore, we applied the method of MAPCURVES to associate individual phenoregions with maps of biomes, land cover, and expert-derived ecoregions. By applying spatial overlays with various maps, this "label-stealing" method exploits the knowledge contained in other maps to identify properties of our statistically derived phenoregions.



3D Virtual Vehicle

Sreekanth Pannala and John Turner

Advances in transportation technologies, sensors, and onboard computers continue to push the efficiency of vehicles, resulting in an exponential increase in design parameter space. This expansion spans the entire vehicle and includes individual components such as combustion engines, electric motors, power electronics, energy

Events [Continued]

storage, and waste heat recovery, as well as weight and aerodynamics. The parameter space has become so large that manufacturers do not have the computational resources or software tools to optimize vehicle design and calibration. This expanded flexibility in vehicle design and control, in addition to stringent CAFE standards, is driving a need for the development of new high-fidelity vehicle simulations, optimization methods, and self-learning control methods.

The biggest opportunity for improvements in vehicle fuel economy is improved integration and optimization of vehicle subsystems. The current industry approach is to optimize individual subsystems using detailed computational tools and to optimize the vehicle system with a combination of low order map-based simulations with physical prototype vehicles. Industry is very interested in reducing the dependence on prototype vehicles due to significant investment cost and time. With increasingly aggressive fuel economy standards, emissions regulations, and unprecedented growth in vehicle technologies, the current approach is simply not sufficient to meet these challenges. The increase in technologies has led to an exponential growth in parameter and calibration space. Advanced modeling and simulation through virtual vehicle framework can facilitate accelerated development of vehicles through the rapid exploration and optimization of parameter space, while providing guidance to more focused experimental studies. Each of the component areas require HPC resources, and an integrated system approach will likely approach Exascale.

Networking and Communications Research and Development

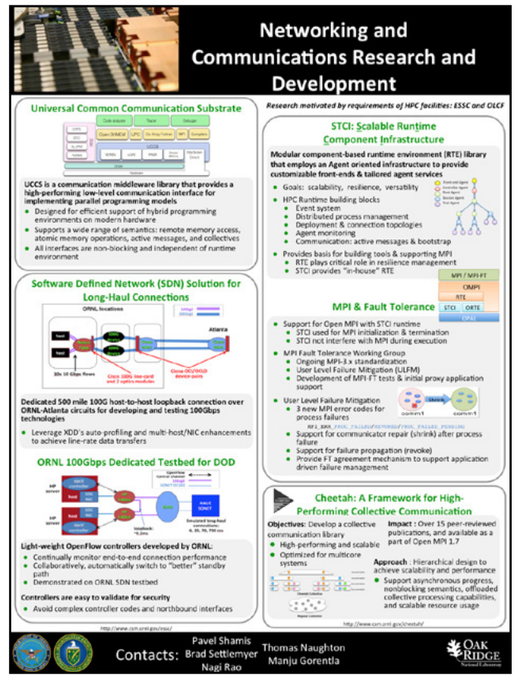
Pavel Shamis, Brad Settlemyer, Nagi Rao, Thomas Naughton, and Manju Gorentla

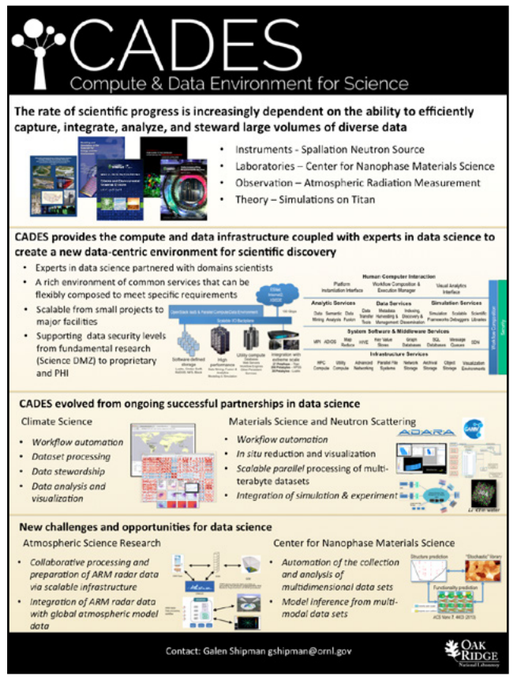
Universal Common Communication Substrate (UCCS) is a communication middleware that aims to provide a high performing low-level communication substrate for implementing parallel programming models. UCCS aims to deliver a broad range of communication semantics such as active messages, collective operations, puts, gets, and atomic operations.

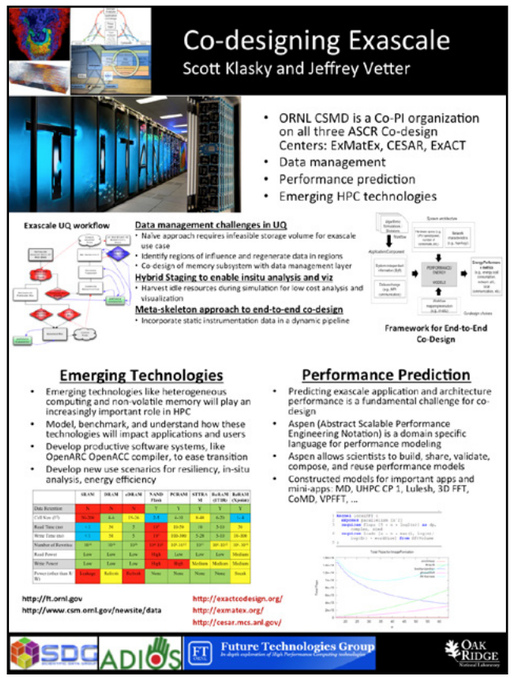
This enables implementation of one-sided and two-sided communication semantics to efficiently support both PGAS (OpenSHMEM, UPC, Co-Array Fortran, ect) and MPI-style programming models.

The interface is designed to minimize software overheads, and provide direct access to network hardware capabilities without sacrificing productivity. This was accomplished by forming and adhering to the following goals:

- Provide a universal network abstraction with an API that addresses the needs of parallel programming languages and libraries.
- Provide a high-performance communication middleware by minimizing software overheads and taking full advantage of modern network technologies with communication-offloading capabilities.
- Enable network infrastructure for upcoming parallel programming models and network technologies.







Compute and Data Environment for Science (CADES)
Galen Shipman

The Compute and Data Environment for Science (CADES) provides R&D with a flexible and elastic compute and data infrastructure. The initial deployment consists of over 5 petabytes of high-performance storage, nearly half a petabyte of scalable NFS storage, and over 1000 compute cores integrated into a high performance ethernet and InfiniBand network. This infrastructure, based on OpenStack, provides a customizable compute and data environment for a variety of use cases including large-scale omics databases, data integration and analysis tools, data portals, and modeling/simulation frameworks. These services can be composed to provide end-to-end solutions for specific science domains.

Co-designing Exascale
Scott Klasky and Jeffrey Vetter

Co-design refers to a computer system design process where scientific problem requirements influence architecture design and technology and constraints inform formulation and design of algorithms and software. To ensure that future architectures are well-suited for DOE target applications and that major DOE scientific problems can take advantage of the emerging computer architectures, major ongoing research and development centers of computational science need to be formally engaged in the hardware, software, numerical methods, algorithms, and applications co-design process. Co-design methodology requires the combined expertise of vendors, hardware architects, system software developers, domain scientists, computer scientists, and applied mathematicians working together to make informed decisions about features and tradeoffs in the design of the hardware, software and underlying algorithms.

CSMD is a Co-PI organization on all three ASCR Co-design Centers:

- Exascale Co-design Center for Materials in Extreme Environments (ExMatEx),
- Center for Exascale Simulation of Advanced Reactors (CESAR), and
- Center for Exascale Simulation of Combustion in Turbulence (ExaCT).

Read more about the ASCR Co-design centers [**here**].

OpenSHMEM Workshop
Oscar Hernandez, Pavel Shamis, and Jennifer Goodpasture

The OpenSHMEM workshop for Extreme Scale Systems Center (ESSC) was held in Annapolis, Maryland on March 4-6. This workshop was held to promote the advancement of parallel programming with the OpenSHMEM programming interface and to help shape its future direction.

The OpenSHMEM workshop is an annual event dedicated to the promotion and advancement of parallel programming with the OpenSHMEM programming interface and to helping shape its future direction. It is the premier venue to discuss and present the latest developments, implementation technology, tools, trends, recent research ideas and results related to OpenSHMEM and its use in applications. This year's workshop also emphasized the future direction of OpenSHMEM and related technologies, tools and frameworks. It also focused on future extensions for OpenSHMEM and hybrid programming on platforms with accelerators.

Topics of interest for conference included (but were not limited to):

- Experiences in OpenSHMEM applications in any domain
- Extensions to and shortcomings of current OpenSHMEM specification
- Hybrid heterogeneous or many-core programming with OpenSHMEM and other languages or APIs (i.e. OpenCL, OpenACC, CUDA, OpenMP)
- Experiences in implementing OpenSHMEM on new architectures
- Low level communication layers to support OpenSHMEM or other PGAS languages/APIs
- Performance evaluation of OpenSHMEM or OpenSHMEM-based applications
- Power / energy studies of OpenSHMEM
- Static analysis and verification tools for OpenSHMEM
- Modeling and performance analysis tools for OpenSHMEM and/or other PGAS languages/APIs.
- Auto-tuning or optimization strategies for OpenSHMEM programs
- Runtime environments and schedulers for OpenSHMEM
- Benchmarks and validation suites for OpenSHMEM

The workshop had participation from DoD, DoE Office of Science, and other National Labs such as Argonne National Lab and Sandia National Lab. Visit the site [**here**].

Durmstrang Review

The spring review for the Durmstrang project managed by the ESSC was held on March 25-26 in Maryland. Durmstrang is a DoD/ORNL collaboration in extreme scale high performance computing. The long term goal of the project is to support the achievement of sustained exascale processing on applications and architectures of interest to both partners. Steve Poole, Chief Scientist of CSMD, presented the overview and general status update at the spring review. Benchmarks R&D discussion was facilitated by Josh Lothian, Matthew Baker (left in photo), Jonathan Schrock, and Sarah Powers of ORNL; Languages and Compilers R&D discussion was facilitated by Matthew Baker, Oscar Hernandez, Pavel Shamis (right in photo), and Manju Venkata of ORNL; I/O and FileSystems R&D discussion was facilitated by Brad Settlemyer of ORNL; Networking R&D discussion was facilitated by Nagi Rao, Susan Hicks, and Paul Newman of ORNL; Power Aware Computing R&D discussion was facilitated by Chung-Hsing Hsu of ORNL; System Schedulers R&D discussion was facilitated by Greg Koenig, Tiffany Mintz, and Sarah Powers of ORNL. A special panel on Networking R&D was also convened to discuss best practices and path forward. Panelists included both DoD and ORNL members. The topics of discussion during the executive session of the review included continued funding/growth of the program, task progression, and development of performance metrics for the project.

ORNL Software Expo
Jay Billings and Dasha Gorin

There are programmers, researchers, and engineers all over the ORNL campus developing software or modifying existing programs to better meet either their goals, and/or help others reach theirs. Because we are so spread out, many scientists are unaware of others' projects--possibly missing out on important opportunities to collaborate or otherwise ease their burden. The Computer Science Research Group would like to provide a chance for everyone to come together and remedy this. We will be hosting a poster session in the JICS atrium on Wednesday, May 7th, from 9:00am-12:00pm. Presenters will be showcasing posters and/or live demos of their projects. Anyone working at ORNL, from interns to senior staff members, may register to present a (non-classified) project at www.csm.ornl.gov/expo; the deadline to register is April 16th. Non-presenting attendees do not need to register. Please join us; this is not only a great networking opportunity, but also a celebration of ORNL's diverse programming community!

Events [Continued]

2014 Gordon Research Conference on Batteries
John Turner

On March 9-14, Computational Engineering and Energy Sciences Group Leader John Turner attended the 2014 Gordon Research Conference on Batteries [1] in Ventura, CA. Dr. Turner presented a poster titled "3D Predictive Simulation of Battery Systems" on behalf of the team working on battery simulation, Sreekanth Pannala, Srikanth Allu, Srdjan Simunovic, Sergiy Kalnaus, Wael Elwasif, and Jay Jay Billings. The work was funded through the Vehicle Technologies (VT) program office within the EERE [2] as part of the CAEBAT program [3]. This program, led by NREL and including industry and university partners, is developing computational tools for the design and analysis of batteries. CSDM staff are leading development of the shared computational infrastructure used across the program.

[1] **http://www.grc.org/programs.aspx?year=2014&program=batteries**
[2] DOE Office of Energy Efficiency and Renewable Energy (EERE)
[3] The Computer-Aided Engineering for Batteries (CAEBAT) program (**http://www.nrel.gov/vehiclesandfuels/energystorage/caebat.html**)

Seminar Series

- March 26, 2014 - Steven Wise: Convergence of a Mixed FEM for a Cahn-Hilliard-Stokes System
- March 18, 2014 - Zhiwen Zhang: A Dynamically Bi-Orthogonal Method for Time-Dependent Stochastic Partial Differential Equation
- March 4, 2014 - David Seal: Beyond the Method of Lines Formulation: Building Spatial Derivatives into the Temporal Integrator
- February 21, 2014 - Zhou Li: Harnessing high-resolution mass spectrometry and high-performance supercomputing for quantitative characterization of a broad range of protein post-translational modifications in a natural microbial community
- February 14, 2014 - Celia E. Shiau: Probing fish-microbe interface for environmental assessment of clean energy
- February 6, 2014 - Susan Janiszewski: 3-connected, claw-free, generalized net-free graphs are hamiltonian
- January 30, 2014 - Wei Guo: High order Semi-Lagrangian Methods for Transport Problems with Applications to Vlasov Simulations and Global Transport
- January 28, 2014 - Jeff Haack: Applications of computational kinetic theory
- January 24, 2014 - Roman Lysecky: Data-driven Design Methods and Optimization for Adaptable High-Performance Systems
- January 21, 2014 - Tuoc Van Phan: Some Aspects in Nonlinear Partial Differential Equations and Nonlinear Dynamics
- January 17, 2014 - John Dolbow: Recent advances in embedded finite element methods
- January 16, 2014 - Aziz Takhirov: Numerical analysis of the flows in Pebble Bed Geometries
- January 13, 2014 - Pablo Seleson: Bridging Scales in Materials with Mesoscopic Models
- January 9, 2014 - Gung-Min Gie: Motion of fluids in the presence of a boundary
- January 6, 2014 - Christine Klymko: Central and Communicability Measures in Complex Networks: Analysis and Algorithms

SOS18

On March 17-20, 2014, Jeff Nichols, Al Geist, Buddy Bland, Barney Maccabe, Jack Wells, and John Turner attended the 18th Sandia-Oak Ridge-Switzerland workshop (SOS18) [1]. The SOS workshops are co-organized by James Ang at Sandia National Laboratory, John Turner at ORNL, and Thomas Schulthess at the Swiss National Computing Center.

The theme this year was "Supercomputers as scientific instruments", and a number of presentations examined this analogy extensively. John Turner, Computational Engineering and Energy Sciences Group Leader conveys the following impressions: (1) Python is ubiquitous, (2) Domain Specific Languages (DSLs) are no longer considered exotic, (3) proxy apps / mini-apps continue to gain popularity as a mechanism for domain developers to interact with computer scientists, and (4) there is increased willingness on the part of code teams to consider a full re-write of some codes, but funding for such activities remains unclear.

Presentations can be obtained from the SOS18 web site [2].

[1] **http://www.cscs.ch/sos18/index.html**
[2] **http://www.cscs.ch/sos18/agenda/index.html**

Events [Continued]

Software Productivity for Extreme-Scale Science Workshop

The ASCR Workshop on Software Productivity for Extreme-Scale Science (SWP4XS) was held 13-14 January 2014 in Rockville, MD. The meeting was organized by researchers from ANL, LBNL, LANL, LLNL, ORNL (David Bernholdt, CSR/CSMD), and the Universities of Alabama and Southern California at the behest of the US Department of Energy Office of Advanced Scientific Computing Research, to bring together computational scientists from academia, industry, and national laboratories to identify the major challenges of large-scale application software productivity on extreme-scale computing platforms.

The focus of the workshop was on assessing the needs of computational science software in the age of extreme-scale multicore and hybrid architectures, examining the scientific software lifecycle and infrastructure requirements for large-scale code development efforts, and exploring potential contributions and lessons learned that software engineering can bring to HPC software at scale. Participants were asked to identify short- and long-term challenge of scientific software that must be addressed in order to significantly improve the productivity of emerging HPC computing systems through effective scientific software development processes and methodologies.

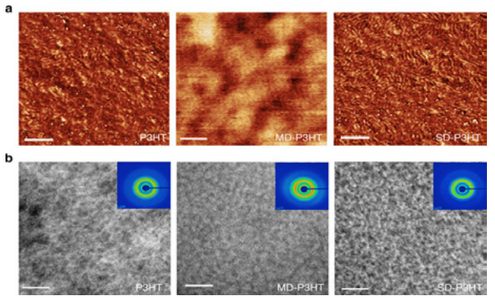
The workshop included more than 70 participants, including ORNL researchers Ross Bartlett (CEES/CSMD), Al Geist (CTO/CSMD), Judy Hill (SciComp/NCCS), Jeff Vetter (FT/CSMD), in addition to organizer Bernholdt. Participants contributed 35 position papers in advance of the workshop, and the workshop itself included 19 presentations, a panel discussion, and three sets of breakout sessions, most of which are archived on the workshop's web site (**http://www.orau.gov/swproductivity2014/**)

An outcome of the workshop will be a report that articulates and prioritizes productivity challenges and recommends both short- and long-term research directions for software productivity for extreme-scale science.

Scientific Achievements

The Isotopic Effects of Deuteration on Optoelectronic Properties of Conducting Polymers
Ming Shao, Jong Keum, Jihua Chen, Youjun He, Wei Chen, James F. Browning, Jacek Jakowski, Bobby G. Sumpter, Ilia N. Ivanov, Ying-Zhong Ma, Christopher M. Rouleau, Sean C. Smith, David B. Geohegan, Kunlun Hong and Kai Xiao

The attractive optoelectronic properties of conducting polymers depend sensitively upon intra- and inter-polymer chain interactions, and therefore new methods to manipulate these interactions are continually being pursued. Here, we report a study of the isotopic effects of deuterium substitution on the structure, morphology and optoelectronic properties of regioregular poly(3-hexylthiophene)s with an approach that combines the synthesis of deuterated materials, optoelectronic properties measurements, theoretical simulation and neutron scattering. Selective substitutions of deuterium on the backbone or side-chains of poly(3-hexylthiophene) s result in distinct optoelectronic responses in poly(3-hexylthiophene)/[6,6]-phenyl-C61-butyric acid methyl ester (PCBM) photovoltaics. Specifically, the weak non-covalent intermolecular interactions induced by the main-chain deuteration are shown to change the film crystallinity and morphology of the active layer, consequently reducing the short-circuit current. However, side-chain deuteration does not significantly modify the film morphology but causes a decreased electronic coupling, the formation of a charge transfer state, and increased electron–phonon coupling, leading to a remarkable reduction in the open circuit voltage. Please read the full document [**here**].



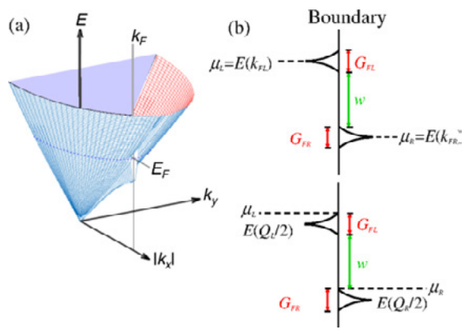
(a) AFM phase images of P3HT, MD-P3HT and SD-P3HT blended with PCBM after thermal annealing (scale bar, 200 nm). (b) Energy-filtered TEM images of P3HT, MD-P3HT and SD-P3HT blended with PCBM after thermal annealing (scale bar, 100 nm). Each film is imaged with 19±4 eV, where inelastic scattering is more intense for P3HT. Insets show the selected area electron diffraction patterns and (c) corresponding integrated diffraction intensity plots of P3HT, MD-P3HT and SD-P3HT blended with PCBM after thermal annealing.

Scientific Achievements [Continued]

Energy Gap Induced by Friedel Oscillations Manifested as Transport Asymmetry at Monolayer-Bilayer Graphene Boundaries

K. W. Clark, X.-G. Zhang, G. Gu, J. Park, G. He, R. M. Feenstra, and A.-P. Li

Electrons, by their quantum nature, are also waves. When scattered by static defects in solids such as metals and semiconductors, they form standing waves that can be seen on the solid surfaces. Such an interference pattern, often called Friedel oscillation, is not expected to impact how electrons conduct in the material because the large electron density can easily dwarf the Friedel oscillation. The situation can be different in materials such as recently discovered graphene and topological insulators, where the electron density is often low and the electronic interaction can become important. In this paper, we demonstrate that the Friedel oscillation can indeed open an energy gap for electron transport in graphene, which in turn can lead to asymmetric transport behavior across the interface in a composite monolayer-bilayer graphene system.



(a) Schematic illustration of the Friedel gap at EF for wave vectors perpendicular to an interface, assuming a linear unperturbed dispersion (e.g., that of graphene). (b) Schematics showing the Friedel gap shifting on two sides of an interface. Upper panel: Friedel gaps open at the respective chemical potentials, without considering the nonequilibrium effect of Friedel gap shifting. Lower panel: Both gaps completely exist below their respective chemical potentials.

Our new finding is that the Friedel gap is opened because the charge oscillation, occurring at the interface, couples the right- and left-going electron waves near the Fermi energy. This gap opens both in the monolayer and in the bilayer of the composite graphene system formed epitaxially on SiC (0001), and it represents an extra energy cost for electron transmission across the monolayer-bilayer interface. The different strengths of the Coulomb interaction in the monolayer and bilayer make their gap sizes different, and that difference is accentuated by the bias voltage and manifested as asymmetric electrical transport across the interface. With our multiprobe scanning-tunneling-potentiometry measurements, we have demonstrated experimentally such a transport asymmetry.

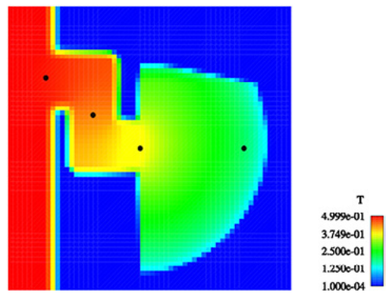
In addition to the fundamental interest of our demonstration of the Friedel-gap-opening phenomenon, the sensitivity of the transport asymmetry to the scattering boundary conditions that we have shown makes scanning-tunneling potentiometry a suitable tool to probe the electron wave functions with respect to their chirality, Berry's phase, and pseudospin polarization.

Please read the full document **[here]**.

A Monte Carlo synthetic-acceleration method for solving the thermal radiation diffusion equation

Thomas M. Evans[1], Scott W. Moshera[1], Stuart R. Slattery[2], Steven P. Hamilton[1]
1 Oak Ridge National Laboratory, 2 University of Wisconsin-Madison

We present a novel synthetic-acceleration-based Monte Carlo method for solving the equilibrium thermal radiation diffusion equation in three spatial dimensions. The algorithm performance is compared against traditional solution techniques using a Marshak bench-mark problem and a more complex multiple material problem. Our results show that our Monte Carlo method is an effective solver for sparse matrix systems. For solutions converged to the same tolerance, it performs competitively with deterministic methods including preconditioned conjugate gradient and GMRES. We also discuss various aspects of preconditioning the method and its general applicability to broader classes of problems.



Two-dimensional plot of the temperature in keV at 1000 ns on a cut-plane positioned at the mid-point of the z-axis.

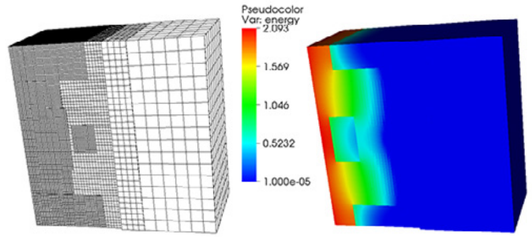
Please read the full document [**here**].

Scientific Achievements [Continued]

Dynamic implicit 3D adaptive mesh refinement for non-equilibrium radiation diffusion

B. Philip[a], Z. Wang[a], M.A. Berrill[a], M. Birke[a], M. Pernice[b]
a Oak Ridge National Laboratory, b Idaho National Laboratory

The time dependent non-equilibrium radiation diffusion equations are important for solving the transport of energy through radiation in optically thick regimes and find applications in several fields including astrophysics and inertial confinement fusion. The associated initial boundary value problems that are encountered often exhibit a wide range of scales in space and time and are extremely challenging to solve. To efficiently and accurately simulate these systems we describe our research on combining techniques that will also find use more broadly for long term time integration of nonlinear multi-physics systems: implicit time integration for efficient long term time integration of stiff multiphysics systems, local control theory based step size control to minimize the required global number of time steps while controlling accuracy, dynamic 3D adaptive mesh refinement (AMR) to minimize memory and computational costs, Jacobian Free Newton–Krylov methods on AMR grids for efficient nonlinear solution, and optimal multilevel preconditioner components that provide level independent solver convergence.



Evolution of AMR mesh and energy on a 16b4l grid on the domain [0, 1] × [0.52, 1] × [0, 1].

Please read the full document [**here**].

New Funding

Fundamental Understanding of Banded Structure Formation during Laser Additive Manufacturing of a Titanium Alloy using Massively Parallel Phase Field Simulations

Principal Investigator: B. Radhakrishnan
Funding Source: ORNL Seed Money Funding

During laser additive manufacturing (LAM), the first-solidified material under the melt pool experiences multiple thermal cycles where the peak temperatures straddle the critical temperatures associated with solid-state transformations. The type, morphology and size scale of the solid-state transformation products are profoundly influenced in a narrow region (~100 mm) in the solidified material, resulting in the formation of a banded structure in commercial titanium alloys that leads to significant anisotropy in the mechanical properties of the final component. The processing history that leads to the formation of the banded structure is not well understood, although it is speculated that short, multiple temperature excursions through phase boundaries are involved. We propose to utilize novel phase field simulations that incorporate transient thermodynamic driving forces and mesoscale strain energy gradients to probe the dissolution, nucleation and growth of second phases during thermal cycling of Ti-6Al-4V. The simulations will help quantify the time-temperature regime under which the bands form, and guide the development of physically based strategies for eliminating the bands in Ti-6Al-4V and potentially other two-phase structural alloys.

Publications and Presentations

Abstract - conference

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- Endeve, Eirik (ORNL), Hauck, Cory D. (ORNL), Xing, Yulong (ORNL), Cardall, Christian Y. (ORNL), Mezzacappa, Anthony (ORNL); Simulating Radiation Transport in Curved Spacetimes, APS April Meeting; Savannah, Georgia
- Evans, Katherine J. (ORNL); Capturing and understanding anomalous events within high resolution climate models, Conference on Data Analytics; Santa Fe, New Mexico 3/2014
- Gaddis, Abigail L. (ORNL), Evans, Katherine J. (ORNL);

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Evaluating high resolution climate model predictability and skill in response to the Mount Pinatubo eruption, 2013 American Geophysical Union Fall Meeting; San Francisco, California 2013

- Humble, Travis S. (ORNL); Quantum Statistical Testing of a Quantum Random Number Generator, SPIE Quantum Communications and Quantum Imaging XII; San Diego, California
- Stoyanov, Miroslav K. (ORNL); Analysis on the Computational Cost of Resilient Methods, SIAM Workshop on Exascale Applied Mathematics Challenges and Opportunities (EX14); Chicago, Illinois 2014
- Sumpter, Bobby G. (ORNL); Computationally Guided Design of Nanostructured Soft Matter and Multicomponent Materials for Energy Science, Electronic Materials and Applications 2014 (American Ceramics Society); Orlando, Florida 1/2014
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Abstract - no conference

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- Mittal, Sparsh (ORNL); Improving Cache Energy Efficiency for Green Computing, Encyclopedia of Business Analytics and Optimization (EBAO), IGI Global, Hershey, Pennsylvania, USA

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