

Upcoming Events

APS Physics

February 27 - March 2
Boston, Massachusetts

The APS March Meeting is the largest physics meeting in the world, focusing on physics research from industry, universities, and major labs.

ACS National Meeting

March 25-29
San Diego, California

If you desire to understand how the chemistry of life impacts your ability to solve many of the most pressing issues within society, then the 243rd ACS National Meeting is the place for you. The theme will focus on advancements in basic and applied research towards understanding the chemistry of life, both at the molecular and macroscopic levels. This meeting boasts more than 11,000 accepted abstracts and promises to be among one of the largest ACS meetings!



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Highlights

CSMD Researcher Receives Secretary of Energy Achievement Honor Award

CSMD researcher Sreekanth Pannala (along with ORNL researchers Charlotte Barbier and David Hetrick) were awarded the Secretary of Energy's Achievement Honor Award. This award is in recognition of their swift and effective response to the Deepwater Horizon oil spill in the summer of 2010.



Secretary Chu and Dr. Pannala

The Flow Rate Technical Group/Nodal Analysis Team, led by Dr. George Guthrie of the National Energy Technology Laboratory and staffed by researchers from NETL, LANL, LBNL, LLNL, PNNL and with support from ORNL and NIST, put forth a multi-agency effort that was critical to estimating the rate of oil flowing into the Gulf and, in turn, develop options to cap the well. The team operated with the utmost efficiency, working tirelessly to assemble, reduce, and analyze data and vet results. Their analyses guided key decisions,

helping speed the ultimate solution and reduce the environmental cost of the disaster.

ORNL Summer Interns Win Scholastic Competition

Oak Ridge High School students Cassee Cain and Ziyuan Liu won the regional championship and a \$6,000 team scholarship at the Siemens Competition in Math, Science and Technology on Saturday at Georgia Tech in Atlanta.



Cassee Cain and Ziyuan Liu

Under the guidance of ORNL biomedical engineers Boyd Evans and John Mueller, Cassee and Ziyuan interned at the Lab during the summer as part of the Oak Ridge High School's math thesis program."

"It has been a wonderful experience working with Cassee and Ziyuan," Boyd said. "They are both impressive and well-rounded students, as well as very grounded as people. Cassee and Ziyuan immediately grasped the importance of the project, as well as the technical requirements."

Highlights (continued)

Cassee and Ziyuan's project involves using Kinect for Xbox 360 and Computer Vision to analyze human gait. The results may aid in the development of an accurate, affordable device to detect abnormal gait patterns.

They will move on to the national competition in Washington, D.C., Dec. 2-5, and a shot at a \$100,000 team scholarship. Ziyuan's father, Bo, works in Computing and Computational Sciences.

The Vols Won SC'11 Best Student Paper Award in Seattle, WA

On November 17, 2011 in Seattle, WA, "Simplified Parallel Domain Traversal," a paper lead-authored by EECS PhD students Wesley Kendall and Jingyuan Wang, won best student paper award at SC'11 conference. Their major adviser is Associate Professor Jian Huang of EECS. The coauthors also include Melissa Allen (CIRES), Dr. Tom Peterka (Argonne National Lab), and CSMD's Dr. David Erickson.

Wes Kendall is supported by Dr. Erickson's NASA proposal and is currently evaluating NASA GCM/Satellite data.

Patent Awarded

CSMD Researcher Travis Humble (along with ORNL researchers Ryan Bennink and Warren Grice) have been awarded a patent for their invention "Tampering Detection System Using Quantum-Mechanical Systems."

According to Dr. Humble, "The patent describes a method for detecting unauthorized physical access to a protected environment. The novelty of the method lies in its use of feedback from a quantum mechanical system to indicate the presence of the intruder. The feedback derives from the non-local correlations, i.e., entanglement, inherent to these systems and the assurance that such measurement signatures can not be spoofed. The ORNL team has experimentally confirmed these ideas using polarization entangled photon pairs as the quantum mechanical probe, and they are currently extending the development of these quantum optical seals for future use in technical verification of nonproliferation treaties."

Software Tools Will Need Refresh for ORNL's Titan Supercomputer

Richard Graham, Group leader for CSMD's/OLCF's Application Performance Tools Group, discusses with HPCWire the challenges presented by new hybrid computer architectures used in Supercomputers such as ORNL's Titan. Read the interview [HERE](#).

Siemens Competition Finalists

Congratulations to Madie Chakoumakos and Tony Zhuang, mentored by CSMD/CCSI researcher Rick Archibald, for being named regional finalists in this year's Siemens Competition in Math, Science, and Technology! Madie and Tony, with the project titled —Characterizing the Elements of the Earth's Radiative Budget: Applying Uncertainty Quantification to Climate Models,|| were among 96 students from 21 states to make it to the regional finals. The Siemens Competition is an annual competition among high school students for college scholarships ranging from \$1,000 to \$100,000.



Tony Zhuang and Madie Chakoumakos

Madie and Tony worked with Rick throughout last summer to characterize the effect of the radiation budget within the Community Earth System Model as various parameters in the Community Atmosphere Model were changed. "Both Madie and Tony were very engaged, energetic, and thoughtful, stated Rick. —I would often walk by their office in Building 6012 and hear their active conversations, as they helped each other come to a greater understanding of the problems. I had to recruit Kate Evans and Bai Yang to help in mentoring just to keep pace with them!"

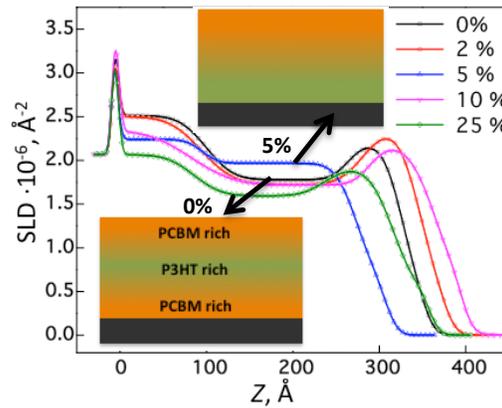
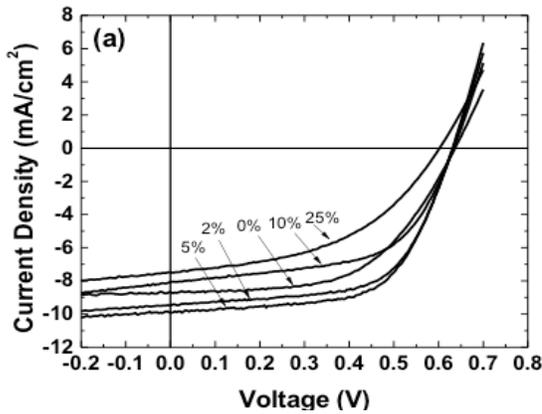
PS-b-P3HT Copolymers as P3HT/PCBM Interfacial Compatibilizers for High Efficiency Photovoltaics

Zhenzhong Sun, Kai Xiao, Jong Kahk Keum , Xiang Yu, Kunlun Hong, Jim Browning, Ilia Ivanov, Jihua Chen, Jose Alonzo, Dawen Li, Bobby Sumpter, Andrew Payzant, Christopher Rouleau, and David Geohegan

This work reports that small amounts (5%) of a tailored diblock copolymer can serve as a compatibilizer to effectively improve the power-conversion efficiency of photovoltaic cells involving blends of polythiophene (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM). At optimal concentrations

Highlights (continued)

the diblock copolymer (PS-*b*-P3HT), which includes an insulating polystyrene (PS) block, was found to induce a highly favorable active layer morphology with interpenetrating nanoscale domains, thus enhancing the overall crystallinity and orientation of the P3HT conducting polymer, and facilitating hole transport within the active layer for higher efficiencies. Neutron reflectivity was used to characterize the phase separation in the polymer blends, and quantum density functional theory calculations were used to understand that the PS-*b*-P3HT diblock copolymer controlled the phase separation of the P3HT and PCBM through strong interactions between the PCBM and the PS block, while the P3HT block induced alignment of the polythiophene.



(a) Electrical characteristics of polymer solar cells with different fractions of diblock copolymer compatibilizers.
(b) Neutron reflectivity data and schematics illustrating how 5% diblock copolymers alter the PCBM distribution within the active layer of the device.

This work was published in *Advanced Materials*, Nov. 18, 2011 DOI:10.1002/adma.201103361. This research was conducted at the Center for Nanophase Materials Sciences, with neutron reflectometry experiment performed on the Liquids Reflectometer at the Spallation Neutron Source, which are user facilities sponsored at Oak Ridge National Laboratory by the Office of Basic Energy Sciences, U.S. Department of Energy.

Awards

Distinguished Employee Program

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

- November 2011: Eric Lingerfelt - For his agile development of the Bellerophon software platform. October's release of Bellerophon (1.1.8) not only included the usual group of bug fixes, etc., but also included significant new functionality to help computational scientists glean insight from simulation. New caching techniques and expanded VisIt functionality through Bellerophon are the chief improvements. These new features have set the stage for the generalization of Bellerophon for other code teams.
- October 2011: Antonios Danalis - For being a Good Samaritan - What happened: I was taking a walk around the pond (only to fight off 2:00 sleepiness so I can be more productive :-)), when I suddenly saw huge sparks and heard violent sounds from behind the trees across the road (where the intersection of the power lines is). Shortly after, I saw a car slowly coming from the electric tower toward the pond, very close to where I was. The car continued through the grass, over the road and into the pond. I couldn't see anybody in the driver's seat, but I assumed that somebody had to be driving this car, so I ran, jumped in the pond, opened the back door that was still above the water, got in the car, saw the lady laying on her side (semiconscious) and started pulling her up and trying to wake her up. Her leg was stuck between the seat and the console, so I couldn't set her free, but another guy helped me open the front door and then we moved the seat back and set her leg free. Soon the fire department, police and paramedics came and they took over. Donna walked away, so she is probably not in too much medical trouble. She was lucky though; given how long it took us to set her free and that she was semiconscious at best, if the pond was deep enough to swallow the whole car, I don't know that we would have managed to get her out in time.

Other Awards/Recognition

Danny McKenna

Danny McKenna was granted the status of Fellow by the Royal Meteorological Society.

Oak Ridge Institutional Cluster Addition

CSMD announces its addition to the Oak Ridge Institutional Cluster (OIC).

At the end of last year, CSMD purchased additional computing power for the OIC. The specifications for this new system are as follows:

- SGI Altix
- Panasas Parallel File System (20TB)
- Infiniband Interconnect Switch (QDR)
- 42 compute nodes, each with dual hexacore hyperthreaded 2.4 GHz Xeon processors (24 hyperthreaded processors/node, 24GB Memory/node)
- Total 1008 processors - 4.91 TFlops

The OIC is a multi-programmatic heterogeneous federated cluster. Supported by ITSD R&D Systems Engineering staff at ORNL, the OIC provides HPC service to several hundred users and many different programs at the laboratory, charging a monthly subscription to unit owners. The OIC currently has a theoretical rating of 36.6 peak TFLOPs across all 18 units. Currently ITSD offers free accounts with limited support on a one unit portion of the "Phase 1" OIC. Submissions to this "ORNL General User" queue and other queues are prioritized based on the Fair Share algorithm with no Incite proposal required. All OIC accounts require users to have ORNL UCAMS accounts. The objective of the OIC is to provide High Performance Computing (HPC) capabilities for ORNL R&D projects in ways that complement and support the broader Leadership Computing Facility (LCF) mission.

If you need to schedule compute time or want to learn more about the OIC, please visit oic.ornl.gov.

New Group Leader for CSMD



In December, Dr. Scott Klasky assumed the role as Group leader of CSMD's Statistics and Data Science Group. Dr. Klasky's previous role at ORNL was as a senior research and development scientist in the Scientific Computing Group within the National Center for Computational Sciences and was the end-to-end task lead in the Oak Ridge Leadership Computing Facility (OLCF).

Dr. Klasky is the leader of the Adaptable I/O System (ADIOS), which includes a large collaboration of researchers from many laboratories and universities. Dr. Klasky is a world leader in the scientific data management community, and has extensive experience working with applications in relativity, astrophysics, combustion, and fusion communities.

Prior to joining ORNL, he was the head of visualization and simulation data management at the Princeton Plasma Physics laboratory. Klasky's tasks at ORNL include working with many of the Fusion SciDAC projects (CEMM, SWIM, GPS, CPES), and developing end-to-end solutions for these projects.

Dr. Klasky received his BS in Physics from Drexel University in 1989. He then received a Ph.D. in physics from the University of Texas at Austin in 1994. The topic of Klasky's thesis was in numerical methods to solve elliptical partial differential equations for numerical relativity. During his time as a student, Klasky also worked as a research assistant at the Center for High Performance Computing at Texas. His work there was in the visualization group, working on developing visualization software for researchers at Texas. After receiving his Ph.D., Klasky became a postdoctoral research associate at Texas, working on advanced computing techniques for the NSF funded grand challenge, "The Binary Black Hole Grand Challenge". Between 1996 and 1999, Klasky became a senior research scientist at the Northeast Parallel Architecture Center at Syracuse University.

Moving On

Vasilios Alexiades

Vasilios Alexiades retired from ORNL in November 2011 after almost 30 years (part-time) in the Math group. He worked primarily on moving boundary problems (phase-change modeling). He continues as professor of Mathematics at UTK, so he will still be attending interesting events at ORNL.

Mark Gomien

Mark Gomien, a nationally recognized expert in missile defense systems analysis, departed to work on a classified effort for a Missile Defense Agency contractor.

Barbara Jackson

Barbara Jackson retired from ORNL effective January 1, 2012 after 43 years at ORNL. Most recently, Barbara was recognized for her outstanding computer programming support of the Environmental Sciences Division's AmeriFlux data base. For the AmeriFlux project, Barbara was responsible for:

- Writing over 1000 SAS codes to read, check, and merge a multitude of data streams from over 40 AmeriFlux site teams
- Assembling the "AmeriFlux Network database," which now contains over 300 million observations and 700 variables
- Developing web documents detailing CDIAC's site-specific QA/QC contributions to the AmeriFlux database
- Creating a web-based interface for users to query the AmeriFlux database
- Producing standardized AmeriFlux data products fundamental to terrestrial climate change modeling and synthesis activities



*Barbara Jackson and Dennis Wolf
at their retirement party.*

Ahmed Khamayseh

Ahmed Khamayseh departed from ORNL on December 31, 2011 for a new professorship position at the Palestine Polytechnic University in Hebron, Palestine. For the last ten years Ahmed was expert resident of mesh generation and computational geometry at ORNL. He was a Co-PI and a key contributor to the Scientific Discovery through Advanced Computing (SciDAC) Terascale Simulation Tools and Technologies (TSTT) and Interoperable Technologies for Advanced Petascale Simulations (ITAPS) project activities that included the developments of new geometry and mesh generation capabilities.

Currently, Ahmed is the chair for organizing the International Palestinian Conference on Modern Trends in Mathematics and Physics www.pcmtmp.org which will be held during 16-18 July 2012 at the Palestine Polytechnic University in Hebron, Palestine.

Dennis Wolf

Dennis Wolf retired from ORNL effective January 1, 2012 after nearly 29 years as a statistical consultant. In 1977 he hired into the Mathematics and Statistics Research Department then located at Y-12. In 1981 he took a 5-year leave of absence to get a PhD in statistics at the University of Wisconsin and in 1986 returned to Computer Science and Mathematics Division at ORNL. Dennis consulted with researchers from diverse application areas. His work with Chemical and Biological Mass Spectrometer (CBMS) team resulted in the first integrated instrument capable of detecting and identifying both chemical and biological warfare agents in the field and earned an R&D 100 Award. He consulted with environmental scientists and geologists applying statistical analyses to understand seasonal and geologic trends in ORNL groundwater and surface water constituents and contaminants. In the SensorNet for Fire and First Responders (SNIFFER) project, he helped the ORNL team fuse a number off-the-shelf chemical sensors into an effective device for detecting toxic industrial chemicals (TICs). In a forensic science project, he employed statistical analyses to relate human decomposition chemistries to time since death (TSD). He also applied multivariate statistical analyses to unexploded ordnance (UXO) surveys to discriminate between ordnance-related and nonordnance-related objects from magnetometer signal transects collected with an airborne platform. Dennis plans to travel and pursue other interests in retirement but expects to retain ties to ORNL.

Community Service



The SuperComputing 2011 (SC11) conference took place this past November in Seattle, Washington. The conference continued a long and successful tradition of engaging the international community in high performance computing, networking, storage and analysis. SC11 will place an emphasis on bringing together communities to facilitate information exchange, discussions, and new collaborations for research and education related to innovating high performance computing applications and advancing scientific discovery and scholarship.

As in previous years, CSMD researchers played a large part in both organizing and participating in the conference.

SC11 Committee Involvement

- System Software Committee Member: Arthur Maccabe, Oak Ridge National Laboratory
- Applications Committee Member: Scott Klasky, Oak Ridge National Laboratory
- Architecture and Networks Committee Member: Rich Graham
- Birds of a Feather Chair: Jeffery A. Kuehn
- Posters Co-Chair: Philip C. Roth
- Architectures/Networks Area Poster Chair: Arthur Maccabe
- Architectures/Networks Committee Member: Collin B. McCurdy
- Tutorials Committee Members: John W. Cobb, Bradley Settlemyer, Jeffrey Vetter and Patrick Worley
- Broader Engagement Committee Member: Rebecca Hartman-Baker
- Broader Engagement Scavenger Hunt Chair: Rebecca Hartman-Baker

Technical Papers

- Simplified Parallel Domain Traversal – David Erickson
- ISABELA-QA: Query-driven Data Analytics over ISABELA-compressed Extreme-Scale Scientific Data – Nagiza F. Samatova and Scott Klasky
- Performance of the Community Earth System Model – Patrick H. Worley

Tutorials

- Scalable Heterogeneous Computing on GPU Clusters - Jeffrey Vetter, Kyle Spafford and Philip Roth
- Big Data Means Your Metadata Must Work – John Cobb

Panels

- Scientific Data on the Path to Exascale: Lessons, Insights and Predictions from 10+ years on the front lines – Nagiza Samatova

Posters

- Scalable Infrastructure to Support Supercomputer Resiliency-Aware Applications and Load Balancing – Terry Jones
- DCA++ Study on Strong Correlated Electron System Case study: Nematic physics in Cuprate – Shi-Quan Su, Thomas Maier, and Michael Summers
- Detection and Correction of Silent Data Corruption for Large-Scale High-Performance Computing – Christian Engelmann
- A Tunable, Software-based DRAM Error Detection and Correction Library for HPC – Christian Engelmann
- A scalable two-phase parallel I/O library with application to a large scale subsurface simulator – Richard Mills

Birds of a Feather

- Scalable Heterogeneous Computing Forum – Jeffrey Vetter
- Computer Architecture Simulation Framework – Stephen Poole

Community Service (continued)

- Next Generation I/O and visualization requirements for in situ processing – Scott Klasky
- Scientific Data on the Path to Exascale: Lessons, Insights and Predictions from 10+ years on the front lines – Steve Poole
- The MPI 3.0 Standard - The Final Stages – Richard Graham
- Developing, Recruiting, and Retaining a Diverse Workforce in HPC – Rebecca Hartman-Baker, Samantha Foley, and Judith Hill
- Women in HPC: Community Building - Rebecca Hartman-Baker, Samantha Foley, and Judith Hill



Workshops

- 2nd SC Workshop on Petascale Data Analytics: Challenges and Opportunities – Scott Klasky
- Scalable Algorithms for Large-Scale Systems – Al Geist and Christian Engelmann

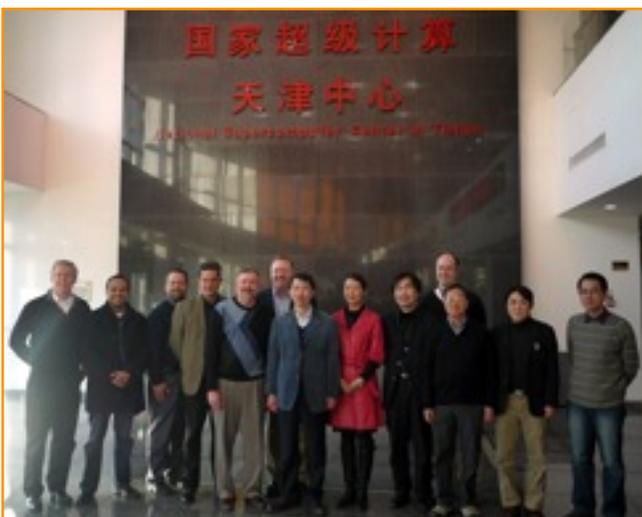
Booth Speaker

- Richard Graham - Titan's programming environment (PE): The challenge of heterogeneity

For SuperComputing 2012, the technical program chair will be Jeffrey Vetter.

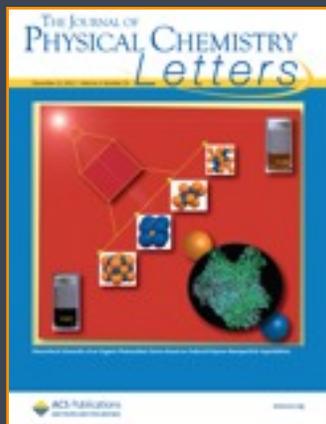
OTHER COMMUNITY SERVICE

- John Cobb, as part of his service on the NEES Governing board, attended the Fall George E. Brown, Jr., Network for Earthquake Engineering Simulation (NEES) governing board meeting at Purdue university on November 22.
- Paul Kent was an Organizing Committee Member for the Conference on Computational Physics 2011, Gatlinburg TN Oct. 30- Nov. 3 (2011).
- Thomas Maier was the Session Chair for Plenary I and V sessions at the Conference on Computational Physics 2011, Gatlinburg, TN Oct. 30- Nov. 3 (2011).
- Bobby Sumpter was the Session Chair for oral session 12.3 “Computational Physics and Sustainable Energy” at the Conference on Computational Physics 2011, Gatlinburg, TN Oct. 30- Nov. 3 (2011).
- Bobby Sumpter was the Chair for the section on “Theory and Algorithms” at the 2011 ASCR/BES Data Workshop, Bethesda, Oct. 24-25 (2011).



Jeffrey Vetter (third from left) at the National Supercomputer Center in Tianjin

- Jeffrey Vetter presented the talk “Critical Role of Software Systems in Exascale Computing” at the Exascale Workshop at the NVIDIA GTC Asia meeting in Beijing. While in Beijing, Jeffrey also visited the Chinese Academy of Sciences to see the Mole-8.5 system and National Supercomputing Center in Tianjin to see Tianhe-1A. The workshop was hosted by Steve Scott of NVIDIA.



Cover Art

The image on the upcoming cover of *The Journal of Physical Chemistry Letters* is from Bobby Sumpter and Anthony Dinsmore's paper "Polymer Nanoparticle Superlattices for Organic Photovoltaic Applications."

Publications/Presentations

Publications

Journal Article

- Annett, James (Trinity College); Gao, Yanfei (ORNL); Cross, Graham (Trinity College); Lucas, Barry N. (Fast Forward Devices, LLC.); Herbert, Erik G. (University of Tennessee, Knoxville (UTK)), *Mesoscale Friction Anisotropy Revealed by Slidingless Tests*, *Journal of Materials Research*, 2373-2378, 26, 18, 9/2011
- Beylkin, Gregory (ORNL); Fann, George I (ORNL); Harrison, Robert J (ORNL); Kurcz, Christopher E (ORNL); Monzon, Lucas A (ORNL), *Multiresolution Representation of Operators with Boundary Conditions on Simple Domains*, *Applied and Computational Harmonic Analysis*, 10, 1, 11/2011
- Chen, Jihua (ORNL); Dadmun, Mark D (ORNL); Mays, Jimmy (ORNL); Messman, Jamie M (ORNL); Hong, Kunlun (ORNL); Britt, Phillip F (ORNL); Sumpter, Bobby G (ORNL); Alonzo Calderon, Jose E (ORNL); Kilbey, II, S Michael (ORNL); Ankner, John Francis (ORNL); Bredas, Jean-Luc E (ORNL); Malagoli, Massimo (ORNL); Deng, Suxiang (ORNL); Swader, Onome A (ORNL); Yu, Xiang (ORNL), *Assembly and Characterization of Well-Defined High-Molecular-Weight Poly(p-phenylene) Polymer Brushes*, *Chemistry of Materials*, 4367, 23, 9/2011
- Chen, Yong (Texas Tech University (TTU)); Zhu, Huaiyu (Illinois Institute of Technology); Roth, Philip C (ORNL); Jin, Hui (Illinois Institute of Technology); Sun, Xian-He (Illinois Institute of Technology), *Global-Aware and Multi-Order Context-Based Prefetching for High-Performance Processors*, *International Journal of High Performance Computing Applications*, 355-370, 25, 4, 11/2011
- Fuentes-Cabrera, Miguel A (ORNL); Orozco, Modesto (Institut de Recerca Biomedica, Parc Cientific de Barcelona, Barcelona, Spain); Luque, Javier (Universitat de Barcelona); Sumpter, Bobby G (ORNL); Blas, Jose (Universidad de Castilla-La Mancha); Ordejon, Pablo J (ORNL); Huertas, Oscar (Universitat de Barcelona); Tabares, Carolina (Universitat de Barcelona), *Structural, Dynamical, and Electronic Transport Properties of Modified DNA Duplexes Containing Size-Expanded Nucleobases*, *Journal of Physical Chemistry A*, 11344, 115, 10/2011
- Fuentes-Cabrera, Miguel A (ORNL), B.H. Rhodes, M.I. Baskes, H. Terrones, J.D. Fowlkes, M.L. Simpson, P.D. Rack, *Controlling the Velocity of Jumping Nanodroplets Via Their Initial Shape and Temperature*, *ACS Nano*, 7130-7136, 5, 9, 2011
- Jia, Jun (ORNL); Liu, Jie (University of California, Irvine), *Stable and Spectrally Accurate Schemes for the Navier-Stokes Equations*, *SIAM Journal on Scientific Computing*, 2421, 33, 5, 2011
- Kent, Paul R (ORNL), Y. Zhang, X. Ke, C. Chen, and J. Yang, *Anomalous Lattice Dynamics near Ferroelectric Instability in PbTe*, *Physical Review Letters*, 175503, 107, 2011
- Kent, Paul R (ORNL), P. Ganesh, V. Mochalin, *Formation, characterization and dynamics of onion like carbon structures from nanodiamonds using reactive force-fields for electrical energy storage*, *Journal of Applied Physics*, 73506, 110, 2011
- Kent, Paul R (ORNL), T. A. Strobel, P. Ganesh, M. Somayazulu, R. J. Hemley, *Novel cooperative interactions and structural ordering in H2S-H2*, *Physical Review Letters*, 2011

Publications/Presentations

- Kent, Paul R (ORNL), P. Ganesh, G. M. Veith, *Role of hydroxyl groups on the stability and catalytic activity of Au clusters on rutile surface*, Journal of Physical Chemistry Letters, 2918, 2, 2011
- Kent, Paul R (ORNL), C. Iacovella, W. French, B. G. Cook, P. T. Cummings, *The role of polytetrahedral structures in the elongation and rupture of gold nanowires*, ACS Nano, 2011
- Kent, Paul R (ORNL), H. Zhou, P. Ganesh, V. Presser, M. C. F. Wander, P. Fenter, D. Jiang, A. Chialvo, J. McDonough, K. Shuford, Y. Gogotsi, *Understanding controls on interfacial wetting at epitaxial graphene: Experiment and Theory*, Physical Review B, 2011
- Linton, Dias (ORNL); Dadmun, Mark D (ORNL); Sumpter, Bobby G (ORNL); Teh, Say-Lee (ORNL), *Controlling Non-Covalent Interactions to Modulate the Dispersion of Fullerenes in Polymer Nanocomposites*, Macromolecules, 7737, 44, 9/2011
- Maier, Thomas A (ORNL), S. Maiti, M. M. Korshunov, P. J. Hirschfeld, and A. V. Chubukov, *Evolution of the Superconducting State of Fe-Based Compounds with Doping*, Physical Review Letters, 147002, 107, 2011
- Maier, Thomas A (ORNL), C. Zhang, M. Wang, H. Luo, M. Wang, M. Liu, J. Zhao, D. L. Abernathy, K. Marty, M. D. Lumsden, S. Chi, S. Chang, J. A. Rodriguez-Rivera, J. W. Lynn, T. Xiang, J. Hu, and P. Dai, *Neutron Scattering Studies of spin excitations in hole-doped Ba_{0.67}K_{0.33}Fe₂As₂ superconductor*, Scientific Reports, 1, 2011
- Maier, Thomas A (ORNL), D. Scalapino, *Pair structure and the pairing interaction in a bilayer Hubbard model for unconventional superconductivity*, Physical Review B, 180513, 84, 2011
- Reuter, Matthew G (ORNL); Hill, Judith C (ORNL); Harrison, Robert J (ORNL), *Solving PDEs in Irregular Geometries with Multiresolution Methods I: Embedded Dirichlet Boundary Conditions*, Computer Physics Communications, 1, 183, 2012
- Sampath, Rahul S (ORNL); Barai, Pallab (ORNL); Nukala, Phani K (ORNL), *A parallel multigrid preconditioner for the simulation of large fracture networks*, Journal of Statistical Mechanics: Theory and Experiment, 1-9, P03029, 3/2010
- Sumpter, Bobby G (ORNL), P. Wu, J. Huang, V. Meunier, R. Qiao, *Complex Capacitance Scaling in Ionic Liquids-Filled Nanopores*, ACS Nano, 9044-9051, 5, 11, 2011
- Sumpter, Bobby G (ORNL), S-L. Teh, D. Linton, M.D. Dadmun *Controlling Non-Covalent Interactions to Modulate the Dispersion of Fullerenes in Polymer Nanocomposites*, Macromolecules, 7737-7745, 44, 2011
- Sumpter, Bobby G (ORNL), Z. Sun, K. Xiao, X. Yu, K. Hong, J.K. Keum, J. Browning, I.N. Ivanov, J. Chen, J. Alonzo, D. Li, A. Payzant, C. Rouleau, D.B. Geohegan, *P3HT-*b*-PS Copolymers as P3HT/PCBM Interfacial Compatibilizers for High Efficiency Photovoltaics*, Advanced Materials, 5529-5535, 23, 2011
- Sumpter, Bobby G (ORNL), J. A. Labastide, M. Baghgar, I. Dujovne, Y. Yang, A.D. Dinsmore, D. Venkataraman, M.D. Barnes, *Polymer Nanoparticle Superlattices for Organic Photovoltaic Applications*, Journal of Physical Chemistry Letters, 3085-3091, 24, 2, 2011 (see Cover Art)
- Sumpter, Bobby G (ORNL); Barnes, Mike D. (University of Massachusetts, Amherst); Venkataraman, Dhandapani (University of Massachusetts, Amherst); Dinsmore, Anthony D (ORNL); Labastide, Joelle (University of Massachusetts, Amherst); Baghgar, Mina (University of Massachusetts, Amherst); Yang, Yipeng (University of Massachusetts, Amherst), *Polymer Nanoparticle Superlattices for Organic Photovoltaic Applications*, Journal of Physical Chemistry Letters, 3085-3091, 2, 24, 12/2011
- Sumpter, Bobby G (ORNL); Fuentes-Cabrera, Miguel A (ORNL), J.R. Blas, O. Huertas, C. Tabares, M. Orozco, P. Ordejón, F.J. Luque, *Structural, Dynamical and Electronic Transport Properties of Modified DNA Duplexes Containing Size-Expanded Nucleobases*, Journal of Physical Chemistry B, 11344-11354, 41, 2011

Publications/Presentations (continued)

- Sumpter, Bobby G (ORNL); Fuentes-Cabrera, Miguel A (ORNL), Q. Li, C. Han, S. Horton, W. Lu, J. Bernholc, P. Maksymovych, M. Pan, *Supramolecular Self-Assembly of π -conjugated Hydrocarbons via 2D Cooperative CH/ π Interaction*, ACS Nano, 2011
- Wang, Yanli (ORNL); Xu, Hanbing (ORNL); ERDMAN III, DONALD L (ORNL); Starbuck, J Michael (ORNL); Simunovic, Srdjan (ORNL), Characterization of High Strain Rate Mechanical behavior of AZ31 magnesium alloy using 3D Digital Image Correlation, *Advanced Engineering Materials*, 943, 13, 10, 2011
- Zheng, Lili (University of Tennessee, Knoxville (UTK)); Gao, Yanfei (ORNL); Lee, Sooyeol (ORNL); Barabash, Rozaliya (ORNL); Lee, Jinhaeng (University of Tennessee, Knoxville (UTK)); Liaw, Peter K (University of Tennessee, Knoxville (UTK)), *Intergranular Strain Evolution near Fatigue Crack Tips in Polycrystalline Metals*, *Journal of the Mechanics and Physics of Solids*, 2307-2322, 59, 11, 11/2011

Abstract - Conference

- Ashfaq, Moetasim (ORNL); Diffenbaugh, Noah (Stanford University), *Near-term, high-resolution, ensemble projections of regional climate*, AGU Fall Meeting, San Francisco, California, 12/2011
- Evans, Kate J (ORNL); Archibald, Richard K (ORNL); Ashfaq, Moetasim (ORNL); Bader, David C (ORNL); Bisht, Gautam (ORNL); Flanery Jr, Raymond E (ORNL); Hack, James J (ORNL); Mahajan, Salil (ORNL); Maltrud, Matthew E. (Los Alamos National Laboratory (LANL)); McClean, Julie L. (Scripps Institute of Oceanography); McKenna, Daniel S (ORNL); Taylor, Mark (Sandia National Laboratories (SNL)); Worley, Patrick H (ORNL), *Mean state and global characteristics of the 1 degree spectral Community Atmosphere Model*, DOE BER Science Team Meeting, Washington, District of Columbia, 9/2011
- Evans, Kate J (ORNL); Archibald, Richard K (ORNL); McKenna, Daniel S (ORNL); Taylor, Mark (Sandia National Laboratories (SNL)); Truesdale, John (National Center for Atmospheric Research (NCAR)); Worley, Patrick H (ORNL), *Development and analysis of a high-resolution spectral Community Atmosphere Model (CAM4)*, DOE BER Science Team Meeting, Washington, District of Columbia, 9/2011
- Jia, Jun (ORNL); Hill, Judith C (ORNL); Fann, George I (ORNL); Evans, Kate J (ORNL); Taylor, Mark (Sandia National Laboratories (SNL)), *A high-order spectral deferred correction time integration method in the CAM-HOMME atmosphere model*, DOE ASCR PI Meeting, Reston, Virginia, 10/2011
- Mukherjee, Partha P (ORNL), *Microstructural modeling of LiFePO₄ granular cathodes: Toward enhanced ion transport*, ECS Meeting, Boston, Massachusetts 2011
- Mukherjee, Partha P (ORNL), *Non-equilibrium Phase Transformation and Particle Shape Effect in Li-ion Battery Materials*, ECS Meeting, Boston, Massachusetts 2011
- Ostrouchov, George (ORNL), *Data and Statistics in High Performance Computing*, 2011 International Conference on Software and Intelligent Information, San Juan, Puerto Rico, 2011
- Radhakrishnan, Balasubramaniam (ORNL); Gorti, Sarma B (ORNL), *Mesoscale Simulation of Grain Boundary - Pore Interactions*, 48th Annual Technical Conference of Society of Engineering Sciences, Evanston, Illinois, 10/2011
- Deiterding, Ralf (ORNL), *Block-structured AMR algorithms for complex hyperbolic applications*, 11/2011

Paper in Conference Proceedings (book, CD, journal)

- Elwasif, Wael R (ORNL); Foley, Samantha S (ORNL); Bernholdt, David E (ORNL); Berry, Lee A (ORNL); Samaddar, D. (ITER Organization, Saint Paul Lez Durance, France); Newman, David E (University of Alaska); Sanchez, R. (Universidad Carlos III, Madrid, Spain), *A Dependency-Driven Formulation of Parareal: Parallel-in-Time Solution of PDEs as a Many-Task Application*, 4th Workshop on Many-Task Computing on Grids and Supercomputers (MTAGS) 2011, Seattle, Washington, 11/2011

Publications/Presentations (continued)

- Jones, Ian S (ORNL); Engelmann, Christian (ORNL), *Simulation of Large-Scale HPC Architectures*, 40th International Conference on Parallel Processing (ICPP) 2011: 2nd International Workshop on Parallel Software Tools and Tool Infrastructures (PSTI), Taipei, 9/2011
- Lifflander, Jonathan (University of Illinois, Urbana-Champaign); Miller, Phil (University of Illinois, Urbana-Champaign); Venkataraman, Ramprasad (University of Illinois, Urbana-Champaign); Arya, Anshu (University of Illinois, Urbana-Champaign); Jones, Terry R (ORNL); Kale, Laxmikant V (University of Illinois, Urbana-Champaign), *Dense LU Factorization on Multicore Supercomputer Nodes*, 26th IEEE International Parallel & Distributed Processing Symposium (IEEE IPDPS 2012), Shanghai, 5/2012
- Perotti, Luigi E. (California Institute of Technology, Pasadena); El Sayed, Tamer (King Abdullah University of Science and Technology (KAUST); Thuwal, Kingdom of Saudi Arabia); Deiterding, Ralf (ORNL); Ortiz, Michael (California Institute of Technology, Pasadena), *Response of fiber reinforced sandwich structures subjected to explosive loading*, 9th International Conference on Sandwich Structures, Pasadena, California, 2011
- Wu, Xing (North Carolina State University); Vijayakumar, Karthik (North Carolina State University); Mueller, Frank (North Carolina State University); Ma, Xiaosong (ORNL); Roth, Philip C (ORNL), *Probabilistic Communication and I/O Tracing with Deterministic Replay at Scale*, 2011 International Conference on Parallel Processing (ICPP 2011), Taipei, 9/2011
- Deiterding, Ralf (ORNL), *Block-structured adaptive mesh refinement - theory, implementation and application*, ESAIM Proceedings, Summer school on multiresolution and adaptive mesh refinement methods, 97-150, 34, Frejus, 12/2011

Presentation Material - Conference

- Agarwal, Pratul K (ORNL), *Evolutionary Conserved Linkage Between Enzyme Fold, Flexibility, and Catalysis*, Zing Conference on Biocatalysis, Puerto Morelos
- Erickson III, David J (ORNL), *Paleometeorology: High resolution Northern Hemisphere wintertime mid-latitude dynamics during the last glacial maximum*, AGU Fall Meeting, San Francisco, California
- Kent, Paul R (ORNL), *Lithium Ion Batteries: Challenges and Opportunities for First Principle Simulation*, Department of Physics, Las Vegas, Nevada
- Kent, Paul R (ORNL), *Towards ab initio models of the solid electrolyte interface and improved accuracy for energy materials*, Frontiers of Transformational Materials Science Seminar, Richland, Washington
- Maier, Thomas A (ORNL), *How does the Hubbard Model guide us in the search for higher-Tc superconductors?*, Condensed Matter seminar, Blacksburg, Virginia
- Maier, Thomas A (ORNL), *How does the Hubbard Model guide us in the search for higher-Tc superconductors?*, Condensed Matter seminar, Gainesville, Florida
- Maier, Thomas A (ORNL), *Progress in the Computational Search for higher-Tc superconductors*, Conference on Computational Physics, Conference on Computational Physics, Gatlinburg, Tennessee
- Maier, Thomas A (ORNL), *Superconductivity in cuprate, organic and iron-based materials: A dynamic cluster quantum Monte Carlo perspective*, Electronic structure of novel materials conference, Tegersee
- Mukherjee, Partha P (ORNL); Pannala, Sreekanth (ORNL); Allu, Srikanth (ORNL); Turner, John A (ORNL), *A Multi-Scale Modeling Framework for Li-Ion Batteries*, Lithium Battery Power Conference, Las Vegas, Nevada
- Sumpter, Bobby G (ORNL), *Computational Exploration and Design of Functional Nanostructured Materials*, Workshop on Modeling and Simulation of Materials in Soft Matter Science, Oak Ridge, Tennessee

Publications/Presentations (continued)

- Sumpter, Bobby G (ORNL), *Computational Insight for Guiding the Design of Nanostructured Materials*, 20th Conference on Current Trends in Computational Chemistry, Jackson, Mississippi
- Sumpter, Bobby G (ORNL), *Computational Physics and Sustainable Energy, Computational Physics and Sustainable Energy*, Gatlinburg, Tennessee
- Sumpter, Bobby G (ORNL), *Design of Nanostructured Materials: Can Computational Science Help?*, East Tennessee American Chemical Society meeting, Oak Ridge, Tennessee
- Sumpter, Bobby G (ORNL), *Exploring Structure-Property-Transport Relationships in Nanoscale Graphitic Systems*, 2nd Annual EPSCoR Workshop, Knoxville, Tennessee
- Sumpter, Bobby G (ORNL), *Guiding the Design of Nanostructured Materials for Efficient Energy Storage, Conversion, and Transmission*, Conference on Computational Physics 2011, Gatlinburg, Tennessee
- Sumpter, Bobby G (ORNL), *Simulation of Polymers in Complex Formulations*, P&G workshop, ORNL, Tennessee
- Sumpter, Bobby G (ORNL), *Theory and Algorithms*, 2011 ASCR/BES Data Workshop, Bethesda, Maryland
- Tock, Yoav (IBM Corporation, Haifa Research Center); Mandler, Benjamin (IBM Corporation, Haifa Research Center); Moreira, Jose (IBM T. J. Watson Research Center); Jones, Terry R (ORNL), *Scalable Infrastructure to Support Supercomputer Resiliency-Aware Applications and Load Balancing*, Supercomputing 2011, Seattle, Washington
- Worley, Patrick H (ORNL); Craig, Anthony (National Center for Atmospheric Research (NCAR)); Dennis, John (National Center for Atmospheric Research (NCAR)); Mirin, Arthur A. (Lawrence Livermore National Laboratory (LLNL)); Taylor, Mark (Sandia National Laboratories (SNL)); Vertenstein, Mariana (National Center for Atmospheric Research (NCAR)), *Computer Performance of the Community Earth System Model, Climate and Earth System Modeling (CESM)*, Principal Investigators' Meeting, Washington, District of Columbia

Presentation Material - No Conference

- Baker, Christopher G (ORNL), *Incorporating Trilinos Data Classes into an Application*
- Hauck, Cory D (ORNL), *Optimization-Based Moment Closures in Kinetic Theory and Transport*
- Sullivan, Blair D (ORNL); Groer, Christopher S (ORNL), *Solving Large Graph Problems Using Tree Decompositions: A Computational Study*

Other

- Berrill, Mark A (ORNL); Philip, Bobby (ORNL); Sampath, Rahul S (ORNL); Allu, Srikanth (ORNL); Barai, Pallab (ORNL); Cochran, Bill (ORNL); Clarno, Kevin T (ORNL); Dilts, Gary A (ORNL), *Fiscal Year 2011 Infrastructure Refactorizations in AMP 2011*
- Bernholdt, David E (ORNL), *A Roadmap for NEAMS Capability Transfer*, 11/2011
- Lifflander, Jonathan (University of Illinois, Urbana-Champaign); Miller, Phil (University of Illinois, Urbana-Champaign); Venkataraman, Ramprasad (University of Illinois, Urbana-Champaign); Arya, Anshu (University of Illinois, Urbana-Champaign); Jones, Terry R (ORNL); Kale, Laxmikant V (University of Illinois, Urbana-Champaign), *Exploring Partial Synchrony in an Asynchronous Environment Using Dense LU*, 8/2011

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Group Profile

Computational Earth Sciences

The Computational Earth Sciences Group conducts research in computational methods for the prediction of global and regional climate. An emphasis is placed on the atmospheric dynamics and hydrology of earth systems.

Group Projects

- DOE Biological and Environmental Research Climate Change Prediction Program and the DOE Office of Science SciDAC Program
 - A Scalable and Extensible Earth System Model
 - Earth System Grid
- DOE Office of Science SciDAC Program
 - Multiscale Subsurface Reactive Flows
 - Performance Engineering for the Next Generation Community Climate System Model
- NASA Carbon Assimilation for the Orbiting Carbon Observatory
- USDA Ecosystem Modeling
- ORNL LDRD - Economic modeling and climate feedbacks
- LDRD - Assessing Decadal Prediction of the Earth System after major volcanic eruptions

Research Sponsors

- The current Earth System Modeling projects are sponsored by the DOE Office of Science SciDAC Program. This program is titled Scientific Discovery through Advanced Computing, is exploring and developing the third leg of modern science - simulation - as a paradigm complementing experiment and theory. Funding for these projects is primarily for model development and comes from the DOE Office of Biological and Environmental Research, Climate Research Division.
- The application of the models falls into the applied earth sciences area and takes on a variety of forms requiring specialized techniques of data assimilation, and data analysis. Our sponsors for this area are NASA Earth Missions as well as DOE OBER.
- Mathematical aspects of our modeling work are partially sponsored by the Office of Advanced Scientific Computing Research
- Work on GCM Downscaling and Economic Impacts is supported by the ORNL LDRD program.



About CSMD

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

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

The Division is composed of 10 of Groups. These Groups and their Group Leaders are:

- Computer Science Research - Al Geist
- Future Technologies - Jeff Vetter
- Application Performance Tools - Richard Graham
- Computational Engineering and Energy Sciences - John Turner
- Computational Mathematics - Ed D'Azevedo (Interim)
- Statistics and Data Science - Scott Klasky
- Computational Earth Sciences - Danny McKenna
- Computational Astrophysics - Tony Mezzacappa
- Complex Systems - Jacob Barhen
- Computational Chemical and Materials Sciences - Bobby Sumpter

About this Newsletter

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

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

Contact Information and Links

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LINKS

Computer Science and Mathematics Division - www.csm.ornl.gov

Computing and Computational Sciences Directorate - computing.ornl.gov

Oak Ridge National Laboratory - www.ornl.gov