



### Preparing for the Future of Computational Biology

*Bio-molecular Simulations on Future Computing Architectures* was a workshop held September 16-17, 2010 in the JICS auditorium to discuss the promises and challenges of using computational biology simulations on next-generation computing hardware. Particularly important is the wide-spread availability of graphical processing units (GPUs), and radical change is expected as the transition is made to massively multi-core CPUs and heterogeneous computing environments. Bio-molecular simulations are now used as a routine part of biological research, and can provide vital insights into the working of the cellular machinery at the molecular level.

The workshop brought together over 40 researchers from academic institutions in the U.S. and Europe, hardware vendors (including Cray, NVIDIA, Mellanox, and High Performance Fortran Associates), and DOE laboratories; they included hardware architects, code developers, a variety of users of the molecular modeling techniques and software, biochemists, and biophysicists. Nineteen speakers, including **Pratul Agarwal** and **Al Geist**, presented their work on the changing paradigm of computing hardware and how the bio-molecular simulations continue to benefit from the tremendous increase in computing power. Developers of popular codes – including NAMD, LAMMPS, VMD, GROMACS, ACEMD, OpenMM – discussed ongoing progress, particularly in the ability to routinely model bio-molecules at microsecond time-scale, a long-standing challenge.

Three round-table discussions allowed all the researchers to have interactive discussions, during which they tried to envision what both supercomputers as desktops will operate in 2020, and considered methods, such as the use of GPUs and low-power processors, for improving the quality of bio-molecular simulations.

For more information, see <http://www.csm.ornl.gov/workshops/biomolecular/>.

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### Thesis Defense on the Nile

Omar Sallah was awarded (July 2010) a PhD in Engineering Mathematics from Zagazig University, Egypt. His dissertation, entitled *Mathematical Analysis of Cracked Functionally Graded Plate Materials*, was written at ORNL and **Len Gray** was a member of his committee.

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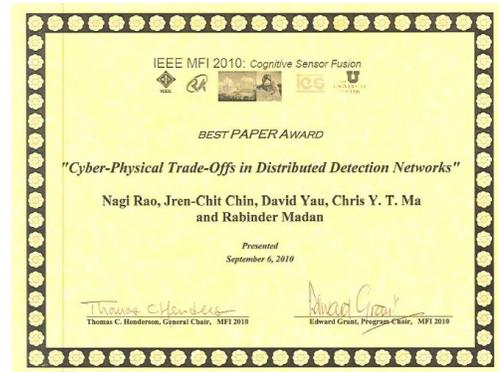
## Outstanding!

Congratulations to **Pratul Agarwal** and his co-authors for winning the “Outstanding Paper Award” at the HPCS 2010, held June 28 - July 2, 2010, in Caen, France.

Hampton, S., Agarwal, P.K., Alam, S.R., and Crozier, P.S. “Towards microsecond biological molecular dynamics simulations on hybrid processors”. *Proceedings of the 2010 International Conference on High Performance Computing and Simulation*, p. 98-107.

## Best Paper at IEEE Conference

**Nagi Rao**, a CSMD Corporate Fellow, and his coauthors from Purdue University and the Office of Naval Research, received the best paper award at the 2010 IEEE International Conference in Multisensor Fusion and Integration, held September 5-7, 2010, in Salt Lake City. This work was funded by DOE ASCR Applied Math Program: Mathematics of Complex Networks.



Nageswara S. V. Rao, Jren-Chit Chin, David K. Y. Yau, Chris Y. T. Ma, and Rabinder Madan. "Cyber-Physical Trade-Offs in Distributed Detection Networks". *Proc. IEEE Int'l Conf. Multisensor Fusion and Integration for Intelligent Systems (MFI)*, Salt Lake City, Utah, September 2010.

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## Conferences

### TeraGrid '10

Attendance at the Annual TeraGrid conference (this year in Pittsburgh, PA) exceeded 400, including over 100 students. ORNL's effort for TeraGrid, the Neutron Science TeraGrid Gateway – a collaboration between CSMD and SNS – was well-represented – as were other ORNL partner TeraGrid projects such as Georgia Tech's Keeneland project and UT's RDAV and NICS projects. Some highlights of the conference were a lively panel on cyber-infrastructure integration across many large NSF science projects (such as iPlant, OOI, LIGO, and NEES), a technology track paper overview of the NSF DataONE datanet project, and a BoF on the datanet program in general.

For more information, see <https://www.teragrid.org/web/events/tg10>.

### SciDAC 2010

The Scientific Discovery through Advanced Computing, or SciDAC, program holds an annual conference; this year's was held July 11-15 in Chattanooga and brought together more than 350 scientists for four days of technical and scientific talks, poster sessions and informal discussions, and was chaired by ORNL's Deputy Director for Science and Technology, Thomas Zacharia. Several CSM researchers gave talks or led posters at the conference, and many more contributed to the research efforts covered in

those presentations. To get some idea of the diversity and depth of CSM's participation, please take a look at [http://computing.ornl.gov/workshops/scidac2010/agenda\\_posters.shtml](http://computing.ornl.gov/workshops/scidac2010/agenda_posters.shtml).

## SciApps

About 70 researchers working on some of the nation's most pressing scientific missions gathered at ORNL for the Scientific Applications (SciApps) Conference and Workshop August 3-6. An interdisciplinary team of computational scientists shared experiences, best practices, and knowledge about how to sustain large-scale applications on leading high-performance computing systems while looking toward building a foundation for exascale research.

SciApps 2010 was funded by the Recovery Act. The OLCF's Scientific Computing Group Leader Ricky Kendall and Director of Science Doug Kothe co-hosted the conference. CSM was well-represented; check out the agenda at <http://www.nccs.gov/user-support/training-education/workshops/sciapps-10/> to get an idea of the participants and the topics they covered.

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## 9th Governor's Chair



**Brian Wirth**, an authority in the ways materials behave in extreme environments, has been named the ninth UT-ORNL Governor's Chair, specifically in computational nuclear engineering. He has appointments in both CSMD and the Department of Nuclear Engineering in the College of Engineering at UT-K, and comes to Tennessee by way of UC Berkeley and, previously, Lawrence Livermore National Laboratory. He received a Bachelor's degree in nuclear engineering in 1992 from the Georgia Institute of Technology in 1992, and a Ph.D. in mechanical engineering in 1998 from the UC Santa Barbara, where he was a DOE Nuclear Engineering Graduate Fellow.

Using high-fidelity computation modeling, Wirth investigates the physical processes that are responsible for causing defects in materials and degrading the performance and lifetime of nuclear reactor components. He expects this research to lead to improved prediction of the longevity of nuclear reactor components and ultimately the development of high-performance, radiation resistant materials for advanced nuclear fission and fusion energy applications.

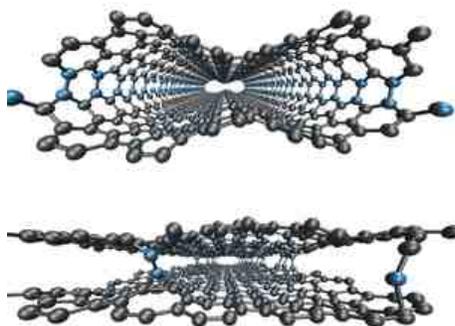
The UT-ORNL Governor's Chair program is designed to attract exceptionally accomplished researchers from around the world to boost joint research efforts. In the words of Governor Phil Bredesen, "Over time, the Governor's Chair program has brought together a diversity of expertise that well represents the goals we set for it. Attracting top scientists and researchers like Brian Wirth as Governor's Chairs continues to broaden and enhance the unique partnership that exists between the University of Tennessee, as the state's flagship university and ORNL, the country's largest multi-program laboratory."

## Computational Chemical Sciences Trifecta

### Graphene Mystery Solved

A research team led by CSM's **Bobby Sumpter**, **Vincent Meunier** and **Eduardo Cruz-Silva** has discovered how loops develop in graphene, an electrically conductive high-strength low-weight material that resembles an atomic-scale honeycomb. Structural loops that sometimes form during a graphene cleaning process can render the material unsuitable for electronic applications. Overcoming these types of problems is of great interest to the electronics industry. The team used quantum molecular dynamics to simulate an experimental graphene cleaning process, as discussed in a paper published in *Physical Review Letters*. Calculations performed on ORNL supercomputers pointed the researchers to an overlooked intermediate step during processing. Imaging with a transmission electron microscope, or TEM, subjected the graphene to electron irradiation, which ultimately prevented loop formation. The ORNL simulations showed that by injecting electrons to collect an image, the electrons were simultaneously changing the material's structure.

The research builds on findings discussed in a 2009 *Science* paper (Jia *et al.*), where Meunier and Sumpter helped demonstrate a process that cleans graphene edges by running a current through the material in a process known as Joule heating. Graphene is only as good as the uniformity or cleanliness of its edges, which determine how effectively the material can transmit electrons. Meunier said the ability to efficiently clean graphene edges is crucial to using the material in electronics.



Recent experimental studies have shown that the Joule heating process can lead to undesirable loops that connect different graphene layers. The PRL paper provides an atomistic understanding of how electron irradiation from a transmission electron microscope affects the graphene cleaning process by preventing loop formation.

See the Publications section of this newsletter for the full citation.

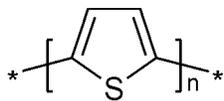
*Especially apropos considering the recent award of the 2010*

*Nobel Prize in physics!*

### “Virtual microscopy” of Pedot

**Bobby Sumpter** and **Vincent Meunier** used computational simulations to help demonstrate and understand epitaxial growth in polymers, foreshadowing a plastic chip process that could combine the high speed of silicon with the low cost of plastic. The research team included scientists from Université du Québec and McGill University in Canada.

The conductive polymer called Pedot (polythiophene) is already widely used in LEDs, displays and solar cells, but not in a crystalline form. Demonstrating epitaxial growth of Pedot could lead to improved, inexpensive organic semiconductors with much better energy efficiency and performance. Sumpter and Meunier collaborated in the project by analyzing the results through a “virtual microscope.” Based on



density functional theory calculations and simulations performed on ORNL supercomputers, the “virtual microscopy” revealed the highly organized structure of the polymer arrays. By examining the polymer formation with the conventional means of scanning tunneling microscopy combined with the virtual microscopy, the team was able to clearly illustrate the construction and bonding of Pedot arrays.

See the Publications section of this newsletter for the full citation.



### Cover Image for *Journal of Materials Research*

Bobby Sumpter reports that a figure from a paper he co-authored (with two other CSM staff members, among others) was selected to be the cover image for the August, 2010 *Journal of Materials Research* focus issue on Materials for Electrical Energy Storage – from “Effect of diffuse layer and pore shapes in mesoporous carbon supercapacitors.”

The CSM trio also had another paper in the same issue – check out the Publications section in this newsletter for full citations.



### Recognition in (Very) Diverse Fields

On the basis of his contributions to open source vehicle routing software, **Chris Groer** was nominated for Full Membership in the COIN-OR Foundation (COmputational INfrastructure for Operations Research), a repository of open source software for optimization and operations research. For more information about the COIN-OR project see <http://www.coin-or.org>.

On a rather different note, Chris has also been selected for induction into the Vanderbilt Sports Hall of Fame, the first male tennis player so honored. He qualified for the NCAA tournament in singles and doubles, became Vandy's first men's All-American in the modern era in 1996, was a two-time Academic All-American, and played on the pro tour for 3.5 years.

## New CMS Group Leader

**Bobby Sumpter** officially became the group leader for Computational Material Science (CMS) on September 1, 2010, after having served as interim group leader over the past year. He will also serve as head of the Nanomaterials Theory Institute in the Center for Nanophase Materials Science. Bobby received his Ph.D. in Physical Chemistry from Oklahoma State University in 1986. After stints at Cornell and UT, he joined the Polymer Science group of ORNL's Chemistry Division in 1992. He has authored or co-authored over 200 publications in refereed journals, and was part of a research team that received the ORNL-CASD Technical Achievement Award in 1996 and the Lockheed Martin Energy Research significant advent award 1999. Not least, his research is featured heavily in this issue of the CSM newsletter.

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## Seismic Shifts in CES

Computational Earth Sciences (CES) not only moved to a new building, but also has a new group leader.

### Moved to 2040

The Computational Earth Sciences Group has moved from the 2<sup>nd</sup> floor of Building 5600 to the 2<sup>nd</sup> floor of Building 2040, better known as the Pro2Serve building. Members of the staff have retained their phone numbers and SAP has been updated to show new room numbers. The CES Group continues its longtime association with the Environmental Sciences and Computer Science Research Groups, and maintains a collaboration area on the 2<sup>nd</sup> floor of 5600. Their new secretary is Deb Holder (576-7433).

Be aware that 2040 is a controlled access building. Enter the reception area at the front of the building, use the phone in the lobby to call your contact, and wait to be escorted to an individual office.

### New Group Leader

**Danny McKenna** joined CSMD as the lead for Computational Earth Sciences Group on September 13, 2010. A native of Scotland, he received Ph.D. in Theoretical Chemistry from the University of Glasgow in 1983. He has served as the Head of the Atmospheric Chemistry Group for the U.K. Meteorological Office; Professor of Physical Chemistry at the University of Bonn, where he was also the founding Director of the Institute for Stratospheric Chemistry and executive director of its parent organization, the Institute for Chemistry and Dynamics of the Geosphere; and Director of the Atmospheric Chemistry Division at NCAR. He is a fellow of the Royal Meteorological Society. In addition to serving as the group leader for CES, Danny will play a key role in defining the relationship between CSMD and the Climate Change Science Institute.

## UTK/ORNL Distinguished Graduate Fellow

Jennifer Ribbeck, one of the first UTK/ORNL Distinguished Graduate Fellows, has begun working with Kate Evans in the Computational Earth Sciences (CES) Group. Under Kate's guidance, she is studying climate models and anticipates making contributions to SEA-CISM, the ice sheet project. The Distinguished Fellowship is a five-year program that combines academic work at UTK and research at ORNL, culminating in a Ph.D. (mathematics in Jennifer's case) and independent, project-supported research at ORNL.

A native Louisianan, Jennifer is now living in Knoxville, having graduated recently from Louisiana State University with a B.S. in mathematics. While at LSU, she worked at the Naval Research Lab at Stennis Space Center, and was awarded not only the LSU University Medal (highest achievable GPA), but also the Betti and Robert Giles Senior Mathematics Award. She presented her undergraduate group's research project at the 2009 SIAM Annual Meeting as a poster entitled, "Resonant Scattering by an Open Waveguide: Dependence on Angle of Incidence and Geometry."

Public service has always been important to Jennifer, and through the Distinguished Fellowship Program, she will have the opportunity to achieve this goal by working at ORNL on scientific applications. She is very excited about being among the first Distinguished Fellows and about joining CSMD.



For more information on this Fellowship Program, see <http://distinguished.utk.edu/>; SEA-CISM info can be found at <http://www.csm.ornl.gov/SEACISM/>.

## Presentations

- **Ralf Deiterding** (*Computational Mathematics*)

**Plenary Lecture:** "Parallel Adaptive Cartesian Upwind Methods for Shock-Driven Multiphysics Simulation." 33<sup>rd</sup> Brazilian National Congress on Applied and Computational Mathematics, Sept. 22, 2010, Aguas de Lindoia, Brazil. ([http://www.congresscentral.com.br/cnmac2010/programa\\_conf.php](http://www.congresscentral.com.br/cnmac2010/programa_conf.php))

## Publications

- Reported by **Kate Evans**:

Evans, K.J., Taylor, M.A., and Drake, J.B. "Accuracy analysis of a spectral element atmospheric model using a fully implicit solution framework". *Monthly Weather Review* **138**:3333-3341 – this work was funded by SciDAC, LDRD, and IAA.

- Reported by **Bobby Sumpter**:

**Jingsong Huang**, Rui Qiao, **Bobby G. Sumpter**, and **Vincent Meunier**. 2010. Effect of diffuse layer and pore shapes in mesoporous carbon supercapacitors. *J. Mater. Res.* **25**: 1469-1475.

**Jingsong Huang**, **Bobby G. Sumpter**, **Vincent Meunier**, Gleb Yushin, Cristelle Portet, and Yury Gogotsi. 2010. Curvature effects in carbon nanomaterials: Exohedral versus endohedral supercapacitors. *J. Mater. Res.* **25**: 1525-1531.

E. Cruz-Silva, A. Botello-Méndez, Z. Barnett, X. Jia, M. Dresselhaus, H. Terrones, M. Terrones, B. Sumpter, V. Meunier. 2010. Controlling Edge Morphology in Graphene Layers Using Electron Irradiation: From Sharp Atomic Edges to Coalesced Layers Forming Loops. *Physical Review Letters*, **105** (4): 045501

J. A. Lipton-Duffin, J. A. Miwa, M. Kondratenko, F. Cicoira, B. G. Sumpter, V. Meunier, D. F. Perepichka, and F. Rosei. 2010. Step-by-step growth of epitaxially aligned polythiophene by surface-confined reaction. *PNAS* **107**: 11200-11204. (see also <http://www.pnas.org/content/107/25/11200.abstract>)

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## Years of Service

Congratulations to the following employees for achieving service milestones!

Richard Archibald ... 5 years

Igor Jouline ... 5 years

Cindy Sonewald ... 5 years

Olaf Storaasli ... 5 years

David Bernholdt ... 10 years

Wael Elwasif ... 10 years

John Cobb ... 15 years

Jacob Barhen ... 25 years

## New Employees

• **Jay Jay Billings**, an astrophysicist and computer scientist, joined **Al Geist's** Computer Science Research (CSR) Group in July. Previously, he held an ORISE post-master's appointment working with **David Bernholdt** on the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. He received his undergraduate degree from Virginia Tech and his Master's degree in Physics from UTK. His current

research is focused on large-scale software design and implementation for energy systems for the complete software lifecycle. He works on the Consortium for the Advanced Simulation of LWRs (CASL), SCALE7, NEAMS, and various other start-up projects.

- **Jingsong Huang** joined the Computational Materials Science Group as a Research Scientist, having worked as a post-doc in Computational Chemical Sciences. Previously, he worked as a Research Fellow at Georgetown University's Chemistry Department.

- **Guruprasad "Guru" Kora** joined the Computer Science Research Group as a Computer Science Researcher; he collaborated with ORNL for many years while working at UT. He received his Master's in Computer Science from Illinois Institute of Technology, with a concentration in Computer Networks. His research focus is Scientific Computing, driven by DOE's HPC, Bioenergy, and Bioremediation mission for fundamental and applied research linked with computational biology.

- **Salil Mahajan**, a summer intern from 2007, has joined the Computational Earth Sciences Group as a Climate Computational Scientist. Previously, he worked as a postdoctoral researcher/visiting scientist in the Atmospheric and Oceanic Sciences Program at Princeton University/Geophysical Fluid Dynamics Laboratory.

- **Pavel "Pasha" Shamis** is a Software Developer in the Application Performance Tools Group. He lived in Haifa, Israel before coming to ORNL, and worked for 10 years at Mellanox Technologies, as an HPC Developer.

## Departures

- **Vincent Meunier**, after almost nine years at ORNL, went to Rensselaer Polytechnic Institute in July as Gail and Jeffrey L. Kodosky '70 Constellation Professor of Physics, Information Technology, and Entrepreneurship. He earned his Ph.D. in physics from Namur University in Belgium in 1999, and put in a stint at North Carolina State University before joining ORNL in 2002. He left as a Senior R&D staff member in the Computational Chemical Sciences Group, and had joined the Nanoscience Theory Institute (NTI) at the Center for Nanophase Materials Sciences (CNMS) in 2005. His work with **Bobby Sumpter** is featured in this issue.

- **Bill Shelton**, a Distinguished Senior Research Staff Member with the Computational Chemical Sciences Group who joined CSM in 1992, was named associate director for Molecular Science Computing at PNNL's Environmental Molecular Sciences Laboratory (EMSL), where he will manage EMSL's high-performance computing capability, including the Chinook supercomputer. Among his accomplishments, he won three Gordon Bell Awards, a Computerworld Smithsonian Award, and three Supercomputing High Performance Computing Challenge Awards.

- **Petr Plechac**, a joint faculty member of UTK and ORNL through JICS, has accepted a professorship at the University of Delaware. He had also been a member of the member of CSM's Computational Mathematics Group.

## Summer Students

The Computer Science and Mathematics Division hosted over seventy summer students this year (students' names are listed followed by their mentors).

Joylika Adams .....	Barhen	Matthew Koehler .....	Groer
Albrecht Albrecht .....	Scott	Jitendra Kumar .....	Mills
Georgios Arabatzis .....	Plechac	Cheuk Ting Li .....	Wong
Woody Austin .....	Meunier	Linus Liang .....	Meunier
Samantha Benham .....	Goswami	Walker Loggins .....	Pouchard
Wesley Bland .....	Graham	Tsz Kin Mak .....	Wong
Cullin Brown .....	Goswami	Alex McCaskey .....	Bernholdt
Jonathan Bryan .....	Meunier	James McClure .....	Graham
George Butler .....	Erickson	Fei Meng .....	Vazhkudai
Chi Po Choi .....	Wong	Alvaro Gutierrez .....	Plechac
Jake Choi .....	Pouchard	Rachel Oliver .....	Hauck
Makasa Covin .....	Pannala	Andrew Ortman .....	Scott
Chris Davis .....	D'Azevedo	Ramya Prabhakar .....	Vazhkudai
Wei Ding .....	Graham	RUI Qiao .....	Meunier
Gemma Dove .....	Imam	Xinyu Que .....	Tipparajuv
Rachel Elkins .....	Goswami	Sudharshan Renganathan .....	Pannala
Elizabeth Figueroa .....	Pouchard	Andrew Runciman .....	Pouchard
Rondria Floyd .....	Goswami	Alberto Salvadori .....	Gray
Samantha Foley .....	Bernholdt	Justin Samuels .....	Gray
Alexander Gann .....	Goswami	Adrian Sanchez .....	Bernholdt
Stephen Gray .....	Erickson	Adam Scarborough .....	Engelmann
Jeddidiah Griffin .....	Goswami	Kendrick Schuettler .....	Harrison
Zhen Guan .....	Plechac	Chris Sellers .....	Cobb
Sulman Haque .....	Harrison	Alexandra Smith .....	Harrison
Jarilyn Hernandez .....	Pouchard	Sethuraman Subbiah .....	Gillen
Lenzie Howell .....	Gray	Humberto Terrones .....	Sumpter
Zhibin Huang .....	Sullivan	Jacob Terry .....	D'Azevedo
Abigail Hueske .....	Hauck	Jeffrey Tithof .....	Erickson
Tushar Janefalkar .....	Imam	Cody Vaughn .....	Archibald
Tomislav Janjusic .....	Graham	Umberto Villa .....	Hill
Deirdre Johnson .....	Barhen	Lukasz Wesolowski .....	Jones
Ian Jones .....	Engelmann	Jesse Wright .....	Maccabe
Egwu Kalu .....	Pannala	Lifan Xu .....	Plechac
Mohammed El Kattani .....	Ostrouchov	Leon Zhang .....	Gray
Mouna Kettani .....	Pouchard	Min Zu .....	Wong
Kishor Kharbas .....	Engelmann		

## News from the Directorate

Interesting items outside CSMD that you might have missed ...

### **Al Gore Explores Green Technologies at ORNL**

Former Vice President Al Gore visited Oak Ridge National Laboratory on Aug. 10 in his role as a partner of a venture capital firm providing early-stage investments to accelerate solutions to the climate crisis. Gore, who shared the 2007 Nobel Peace Prize with the Intergovernmental Panel on Climate Change for disseminating knowledge about man-made climate change, was briefed about renewable technologies, nuclear technologies and climate research. His tour included visits to the Spallation Neutron Source, which provides the world's most intense pulsed neutron beam, and the Oak Ridge Leadership Computing Facility, home to the world's fastest supercomputer.

### **Collaboration between eBird, DataONE and TeraGrid gains recognition**

As the NSF DataONE datanet project is ramping up in its first year, it is already creating synergistic connections between data activities that are opening up new scientific opportunities, such as the analysis of bird migration patterns being done by the experimental Science Visualization and Analysis (EVA) working group. ORNL was a co-author with Daniel Fink of the Cornell Lab of Ornithology on a paper presented at the recent TeraGrid '10 conference (*see above*). In the paper, Daniel presented results from the Cornell eBird project's effort to statistically model bird migration patterns. Recently, eBird, DataONE, the ORNL DAAC's MODIS data, and TeraGrid have all come together under the EVA working group to embark on a larger effort to model the migration patterns of several times as many birds over much longer periods of time in order to show how migration patterns are changing over time and how that is correlated with, and affected by, environmental changes – *e.g.* changing land use patterns, weather variability, and climate change. This effort, although only beginning, has already attracted attention, both at the TeraGrid'10 conference, as well as from the science news media.

Find out more at <http://ebird.org/content/ebird/news/ebird-gets-a-supercomputing-kick-from-teragrid> and <http://www.nature.com/news/2010/100810/full/news.2010.395.html>.

### **High School Students Build Their Own Supercomputer - Almost - at OLCF**

For the third straight year, students and teachers from around Appalachia gathered at ORNL this summer for interactive training from some of the world's leading computing experts. The summer camp, a partnership between ORNL and the Appalachian Regional Commission (ARC) Institute for Science and Mathematics, took place July 12-23. The OLCF hosted 10 students from various backgrounds and parts of the region.

Find out more at <http://www.science.doe.gov/ascr/News/NewsRoundup.html>.