

DOE CSGF COMMUNITY

DEPARTMENT OF ENERGY COMPUTATIONAL SCIENCE GRADUATE FELLOWSHIP PROGRAM



SPRING ISSUE 2009

CALENDAR OF EVENTS...

June:

- Transcripts due
- DOE CSGF fellows' posters at SciDAC - June 14
- DOE CSGF Alumni/Fellow Social at SciDAC - June 17

July:

- HPC Workshop – July 13
- Annual Conference – July 14-16, 2009

August/September:

- Classes begin

October:

- DOE CSGF application posted online

November:

- Renewal Begins

December:

- 2010 Practicum Proposals Due

January:

- Renewals Due
- Essay Contest Due

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2009 – 2010 DOE CSGF Fellows Announced

Edward Baskerville
Ecology
University of Michigan

Kathleen Beutel
Computational Chemistry
University of Minnesota

Sanjeeb Bose
Mechanical Engineering
Stanford University

Kurt Brorsen
Physical Chemistry
Iowa State University

Jeffrey Donatelli
Applied Mathematics
University of California, Berkeley

Piotr Fidkowski
Structural/Computational Engineering
Massachusetts Institute of Technology

David (Virgil) Griffith
Theoretical Neuroscience
California Institute of Technology

Tobin Isaac
Computational and Applied Mathematics
University of Texas at Austin

Mark Maienschein-Cline
Physical Chemistry
University of Chicago

Noah Reddell
Computational Plasma Modeling for
Fusion Energy
University of Washington

Troy Ruths
Bioinformatics
Rice University

Samuel Skillman
Astrophysics
University of Colorado at Boulder

Hayes Stripling
Computational Science
Texas A&M University

Travis Trahan
Nuclear Engineering
University of Michigan

Sean Vitousek
Environmental Fluid Mechanics and
Hydrology
Stanford University

Norman Yao
Condensed Matter Physics
Harvard University

Letter from the Editor



Well, it's been another busy spring with the selection of new fellows, renewals, practicum set-ups and preparation for the annual conference.

We have chosen another great class of 16 DOE CSGF fellows. They're listed in this issue, along with their school and area of study. Most will be at the conference, so please in-

troduce yourself and make them feel welcome into our program.

There are 24 fellows out on practicum this year at nine different labs. Inside you'll find a complete list, including lab assignments.

As for the annual conference, we have a lot of new events this year. See the story inside this newsletter and check them out on the conference web site. I look forward to seeing you all and especially to meeting many of you since I was unable to attend last year.

I'd also like to update you about the twiki web site. We have a section for practicum supervisors and coordinators to list different practicum opportunities. We also have a section for fellows to list the kinds of practicums that interest them. The twiki will serve as a place for fellows and practicum supervisors and coordinators to meet up. Please get on the twiki and register for access to these two sites at <http://info.krellinst.org>.

The practicum twiki sites are just a start. We have more planned for online communities, so look for that in the near future!

Thanks, Jeana

New at the Conference

Summer is here with warm weather, sandals and the fellows' annual conference.

This year the conference moves to July from the traditional June dates. But that's not the only thing different. This year we added a day focusing specifically on high-performance computing (HPC), new optional workshops and a fellows' poster contest. We've also invited lab human resource personnel to attend the lab poster session.

The HPC workshop will be Monday, July 13 from 8 a.m. to 5:30 p.m. It will provide a broad introduction to HPC for scientific and engineering research. The major goal is to kick-start the HPC learning process by helping participants understand why they should utilize HPC and how this will benefit their research.

Attendance is required for incoming, first and second year DOE CSGF fellows. All attendees are welcome, but priority for filling remaining spots will be given to third- and fourth-year DOE CSGF fellows, DOE NNSA SSGF fellows and DOE CSGF alumni. Workshop registration will be confirmed by June 15.

New optional sessions added to Wednesday afternoon include:

- DOE CSGF Fellows and Alumni Session: a chance to discuss anything from the fellowship, jobs, practicums, career paths, etc. DOE CSGF alumna Mayya Tokman will moderate this session.

- HPC Roundtable Discussion: an opportunity to discuss topics and questions about high-performance computing. All are welcome to attend. DOE CSGF Program Manager Mary Ann Leung will moderate this session.

- Writing Tips and Traps: How to Compete for a Reader's Time (and Grant Money) is a writing workshop to assist attendees in writing technique and to give tips on grant writing. Instructors are invited guest Randy Black



Aric Hagberg explaining research at Los Alamos National Laboratory during the DOE Lab Poster session 2008 Annual Conference.

from the Office of Research Development at the University of California, Irvine, with assistance from Bill Cannon, Krell's creative director for science media and Tom O'Donnell, Krell's science and technology writer. This will be an interactive and engaging workshop.

Another new resource at the conference is the invited human resource professionals from the national laboratories. We asked them to join us for the DOE Lab Poster session to give the fellows and alumni a chance to network for both practicum and full-time opportunities. The lab poster session isn't just for practicums anymore!

The DOE CSGF Fellows' Poster Contest also is new this year. Details are posted on the conference web site at <http://www2.krellinst.org/csgf/conf/2009/>. Winners will be announced at Thursday's luncheon.

Lopez Chosen for Corporate Service Corps in Ghana



Written by Tasha Lopez

“This program has your name written all over it.” That was one of a dozen e-mails I received from colleagues in July 2007 when IBM announced the Corporate Service Corps as part of its new Global Citizen Portfolio. I was immediately interested in learning more about this corporate version of the Peace Corps and became one of more than 5,600 employees worldwide who applied in 2008. Over the course of the next year, IBM selected about 300.

I have been active in my local community and the global community for years, so I was characteristically optimistic despite the daunting numbers. I also was fortunate to have a fantastic manager who supported my application even though it would mean losing one of his software salespeople for a period of time.

I was ecstatic when my manager called me in November with news that I had been selected. I later learned I was part of an eight-person global team traveling to Ghana in February 2009.

We received new information every week, so we gradually learned where we'd be living (Takoradi, the third largest city in Ghana with about 350,000 people) and our mission. I was one of three people to be assigned to the nonprofit Association of Ghana Industries (www.agighana.org) to consult with two different clients:

- Multiwall Paper Sack enjoyed 20 years as the sole supplier of packaging for the largest cement company in Ghana. A new local competitor and exported sacks had harmed their business model in recent years, so they requested a business review and recommendations.
- Our other client, West-West Agro-Processing, just ended its two-year start-up phase and was looking for assistance to grow. The company processes fresh peppers

into paste. Their business strategy included selling locally and exporting to Europe. The challenges included farming, sales, marketing, packaging, processing and more.

Upon arrival in Ghana, our team met government officials in the capital city of Accra and learned a lot about Ghana, its economy, government and infrastructure. At one point, we lost power and the presenter didn't even flinch. It was a foretaste of what was to come: intermittent power and Internet access. We later drove about five hours to Takoradi and checked into a 15-room hotel that would serve as home for the next month.

Over the next month, our team held meetings, interviewed stakeholders, dove into years of financial data, studied operations, identified strengths and weaknesses, assessed supply chains, researched markets, negotiated with banks, met with suppliers, toured manufacturing facilities, created spreadsheets, learned how to collect useful information in the absence of data, and outlined our findings and recommendations in 40-page documents for each client.

I am pleased to report that we achieved all of our goals and the companies' executives welcomed our recommendations. Executives at one company acted immediately, so we made significant tangible progress before we even left Ghana.

Though we worked full-time, we also had plenty of time for fun. We visited beautiful beaches and attended a traditional baby naming ceremony. We took a weekend trip to the birthplace of Ghana's first president, visited a village accessible only by canoe and built entirely on stilts, and hiked in the largest rainforest in Ghana, where I was attacked by safari ants and still had a fantastic time. I immersed myself in Ghanaian culture, eating only Ghanaian food (with my fingers!) and wearing Ghanaian clothes on Friday and to church on Sunday.

Some of my favorite memories are seeing a goat walk on the sidewalk outside a bank; nearly dancing on a live scorpion; navigating the tiny pathways in Market Circle; being offered a recently killed forest rat (a prized delicacy); and having our clients tell us what our time there meant for them.

I feel honored to have been able to participate in the Corporate Service Corps. It was the best thing I've done in my eight-year IBM career, and it truly was a win-win-win situation. Our clients received high-tech and high-quality assistance; communities benefited from the work we did because nonprofits experienced systemic improvements; IBM gained new insights into emerging markets while creating loyalty among key employees; and IBM workers gained incredible experiences while making new friends around the world.

If you'd like to learn more about my experience in Ghana, www.tashaefualopez.blogspot.com contains pictures, video and blog entries.

**Alumni
Corner**

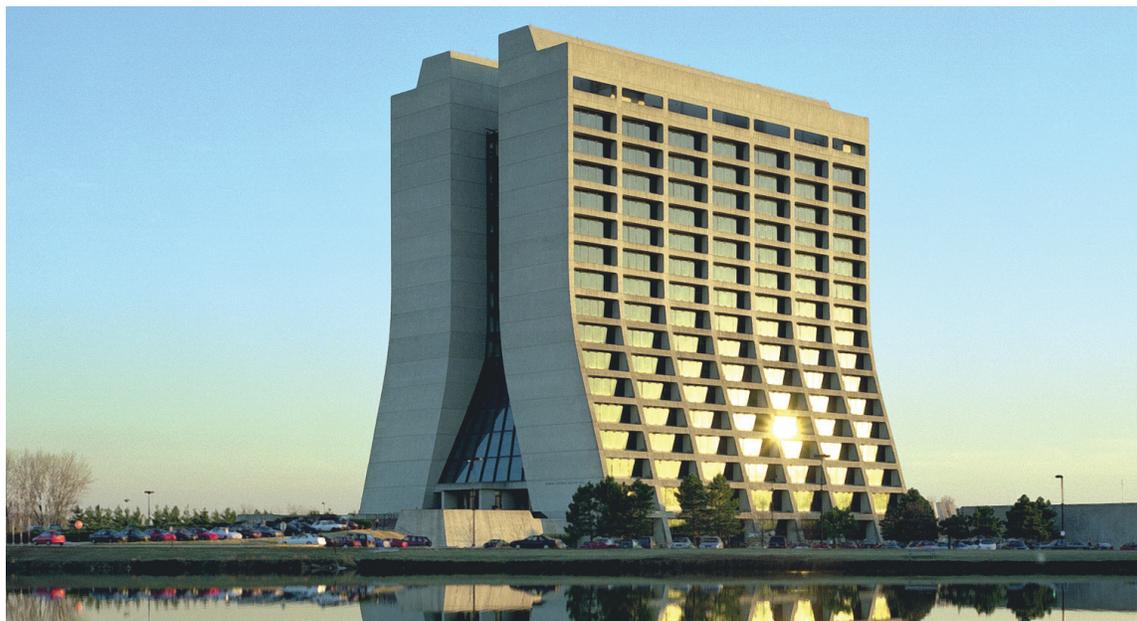
New Practicum Host Sites



National Renewable Energy Laboratory (NREL) Facility of the US Department of Energy (DOE) for renewable energy and energy efficiency research, development and deployment. Courtesy of <http://www.nrel.gov/>

Two new DOE CSGF practicum host sites have been added to our program this spring: The National Renewable Energy Laboratory (NREL) at Golden, Colo., and Fermi National Accelerator Laboratory (Fermilab) at Batavia, Ill. Practicums may be started there as soon as this fall. Representatives from both NREL and Fermilab will attend the DOE Lab Poster Session at the 2009 DOE CSGF Conference. Stop by the NREL and Fermilab booth to learn more about them or find additional information at <http://www.nrel.gov/> and <http://www.fnal.gov/>.

NREL is a mission-focused multidisciplinary laboratory conducting research and development in the biological, chemical, physical and engineering sciences relating to energy efficiency and renewable energy technologies. The Materials and Computational Science Center at NREL maintains a commodity high-performance computing cluster with approximately 8 TFlops of peak performance. Qualified graduate students may use these laboratory resources during the course of their research. NREL's distinctive R&D programs and competencies advance national energy goals by developing innovations to change the way we power our homes and businesses and fuel our vehicles. CSGF fellows performing their practicum at NREL would have the opportunity to work closely with world-leading scientists using state-of-the-art facilities focused on the grand challenge of developing cost-effective renewable energy sources and energy-efficient technologies to meet future demand in an environmentally responsible manner.



Wilson Hall at FermiLab located in Batavia, Illinois. Courtesy of <http://www.fnal.gov/>

Fermilab advances understanding of the fundamental nature of matter and energy by providing leadership and resources for qualified researchers to conduct basic research at the frontiers of high-energy physics and related disciplines. The Fermilab Computing Division has a staff of more than 270, including more than 40 scientists and 180 computing professionals, computer scientists and engineers. Scientists and engineers in other lab divisions and sections collaborate on many computational activities, especially the CMS Physics, Astrophysics and Accelerator centers. The scale and complexity of data in the physics and astrophysics programs provide real-time data acquisition, computational and data challenges that lend themselves to research and development from computer science and related areas of computational research. Programs at Fermilab that already include such activities are accelerator modeling and simulation, advanced scientific workflow, theoretical astrophysics and advanced distributed systems research and development.

2009 Practicum Experiences

ARGONNE NATIONAL LAB –

Practicum Coordinator: Raymond Bair
Zlatan Aksamija, Illinois, Urbana-Champaign
(Paul Fischer)
Kathleen King, Cornell (Sven Leyffer)
Paul Loriaux, UC, San Diego (Kevin White)
Anne Warlaumont, University of Memphis
(Mark Hereld)

BROOKHAVEN NATIONAL LAB –

Practicum Coordinator: James Davenport
Milo Lin, CalTech (James Davenport)

LAWRENCE BERKELEY NATIONAL LAB –

Practicum Coordinator: Daniel Martin
Eric Chi, Rice (Paul Spellman)
Ying Hu, Rice (James Schuck & Jeff Neaton)
Eric Liu, MIT (Phillip Colella)
Douglas Mason, Harvard (Peter Nugent)
Britton Olson, Stanford (Phillip Colella)

LAWRENCE LIVERMORE NATIONAL LAB –

Practicum Coordinator: Jim McGraw
Gregory Crosswhite, Washington
(Jonathan DuBois)
Oaz Nir, MIT (Gabriela Loots)

LOS ALAMOS NATIONAL LAB –

Practicum Coordinator: Aric Hagberg
Scott Clark, Cornell (Nick Hengartner)
Brenda Rubenstein, Columbia (James Gubernatis)

OAK RIDGE NATIONAL LAB –

Practicum Coordinator: James Hack
Joshua Hykes, North Carolina State (Kevin Clarno)
Matthew Norman, North Carolina State
(John Drake)
Alex Perkins, UC, Davis (Yetta Jager)
Matthew Reuter, Northwestern (Robert Harrison)
Paul Sutter, Illinois, Urbana-Champaign
(Robert Harrison)

PRINCETON PLASMA PHYSICS LAB –

Practicum Coordinator: William Tang
Armen Kherlopian, Cornell
(Harry Mynick and Neil Pomphrey)

SANDIA NATIONAL LAB, ALBUQUERQUE –

Practicum Coordinator: Heath Hanshaw
Carolyn Phillips, Michigan (Paul Crozier)
Danilo Scepanovic, Harvard/MIT (Robert Glass)
Cameron Talischi, Illinois, Urbana-Champaign
(Martin Heinstein)

SANDIA NATIONAL LAB, LIVERMORE –

Practicum Coordinator: Alex Lindblad
Curtis Hamman, Stanford (Alan Kerstein)
Ben Sunday, Princeton (Habib Najm)

(Practicum Supervisor)



Fellow Gregory Crosswhite explains his poster during the 2008 DOE CSGF Annual Conference.

Graduating Fellows Take Jobs – Spring '09:

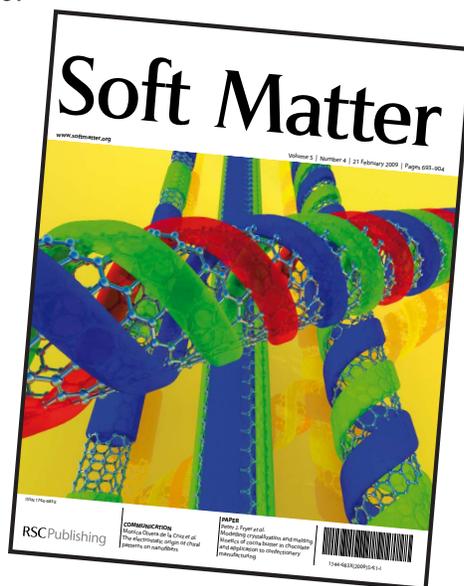
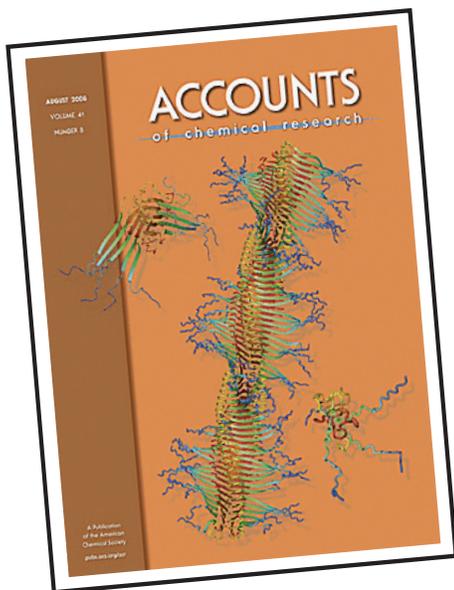
- **JULIANNE CHUNG** received an NSF Mathematical Sciences Postdoctoral Research Fellowship at the University of Maryland at College Park, where she will join Dianne O'Leary's group in the Department of Computer Science.
- **JEFF HAMMOND** successfully defended his thesis in May. On June 1, he starts a Director's Postdoctoral Fellowship at the Argonne Leadership Computing Facility, working with Ray Bair to develop massively parallel quantum chemistry algorithms.
- **DAVID KETCHESON** has accepted an appointment as assistant professor of applied mathematics at King Abdullah University of Science and Technology (KAUST) starting in the fall. David also was awarded an NSF Postdoctoral Fellowship but declined it in order to accept the KAUST appointment.
- **KEVIN KOHLSTEDT** has accepted a postdoctoral position at the University of Michigan starting this fall. He will investigate symmetries of novel colloidal assemblies as part of Sharon Glotzer's group.
- **DAVID MARKOWITZ** has accepted a postdoctoral research job with Bijan Pesaran at the NYU Center for Neural Science starting Sept. 1, 2009. His research will involve massively parallel recordings from cortical neurons during behavior and the development of real-time brain-computer interfaces to support control applications. This could one day allow paralyzed humans to communicate, interact physically with their environment and control wheelchair movement using neural prosthetics.
- **CHRIS SCHROEDER** will start a postdoctoral position at the University of Wuppertal in Germany in January 2010.
- **STEFAN WILD** has been named an Argonne Director's Postdoctoral Fellow at Argonne National Laboratory in the Mathematical and Computer Science Division.

Noteworthy News:

- **Julianne Chung** was a finalist in the SIAM Conference on Computational Science and Engineering student paper competition. She presented her paper at the conference this spring in Miami.

- **Ying Hu** received a 2009 SPIE Scholarship in Optical Science and Engineering.

- **Kevin Kohlstedt** had publications chosen as cover articles in two journals. The first is a review article of Alzheimer's disease research he did during his practicum at Lawrence Berkeley National Laboratory. The cover is an image of an amyloid-beta fibril elongating. See: N.L. Fawzi, E-H. Yap, Y. Okabe, K.L. Kohlstedt, S.P. Brown and T. Head-Gordon, "Contrasting Disease and Nondisease Protein Aggregation by Molecular Simulation." *Acc. Chem. Res.* (2008), 41, 1037. The second article is a summary of work describing how helical patterns wrapped around nanofibers can adopt chiral symmetry, providing a possible explanation for the many chiral filaments seen in biology. The cover image shows the different types of symmetries possible on nanotube surfaces.; See: G. Vernizzi, K.L. Kohlstedt and M.O. de la Cruz, "On the electrostatic origin of chiral patterns on nanofibers." *Soft Matter* (2009), 5, 736.



**Do you have some good news
or a BIG event happening?**

Send your noteworthy news to: gingery@krellinst.org.

- **Carolyn Phillips** was chosen by the Department of Energy to join the U.S. delegation to the 59th Meeting of Nobel Laureates and Students in Lindau, Germany this summer. The meeting will focus on chemistry.

- **Matthew Reuter** was awarded a scholarship from Northwestern University, NSF's Materials Research Science & Engineering Centers and the Weizmann Institute of Science to study complex absorbing potentials and real-space density functional theory at the institute in Rehovot, Israel for five weeks this past winter. He also had a paper appear in *Physical Review Letters* in November: "Laser Field Alignment of Organic Molecules on Semiconductor Surfaces: Toward Ultrafast Molecular Switches," *PRL* 101,208303 (2008). Authors are M.G. Reuter, M. Sukharev and T. Seideman.

- **Sarah Richardson** won a book-collecting contest hosted by the library at her school, Johns Hopkins University School of Medicine.

- **Alex Rodriguez** published a paper on "Stable-suspension and dispersion-induced transitions from repulsive Casimir forces between fluid-separated eccentric cylinders" in *Physical Review Letters*. He also passed his oral qualifying examinations at MIT.



The Department of Energy Computational Science Graduate Fellowship (DOE CSGF) is a program funded by the Department of Energy's Office of Science and National Nuclear Security Administration and administered by the Krell Institute.

Now in its 18th year, the DOE CSGF trains scientists to meet the nation's workforce needs, and creates a nationwide interdisciplinary community. As some of the best scientific graduate students in the nation, the graduates of this unique program now work in DOE laboratories, private industry, educational institutions and many others. For more information, please contact us.

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