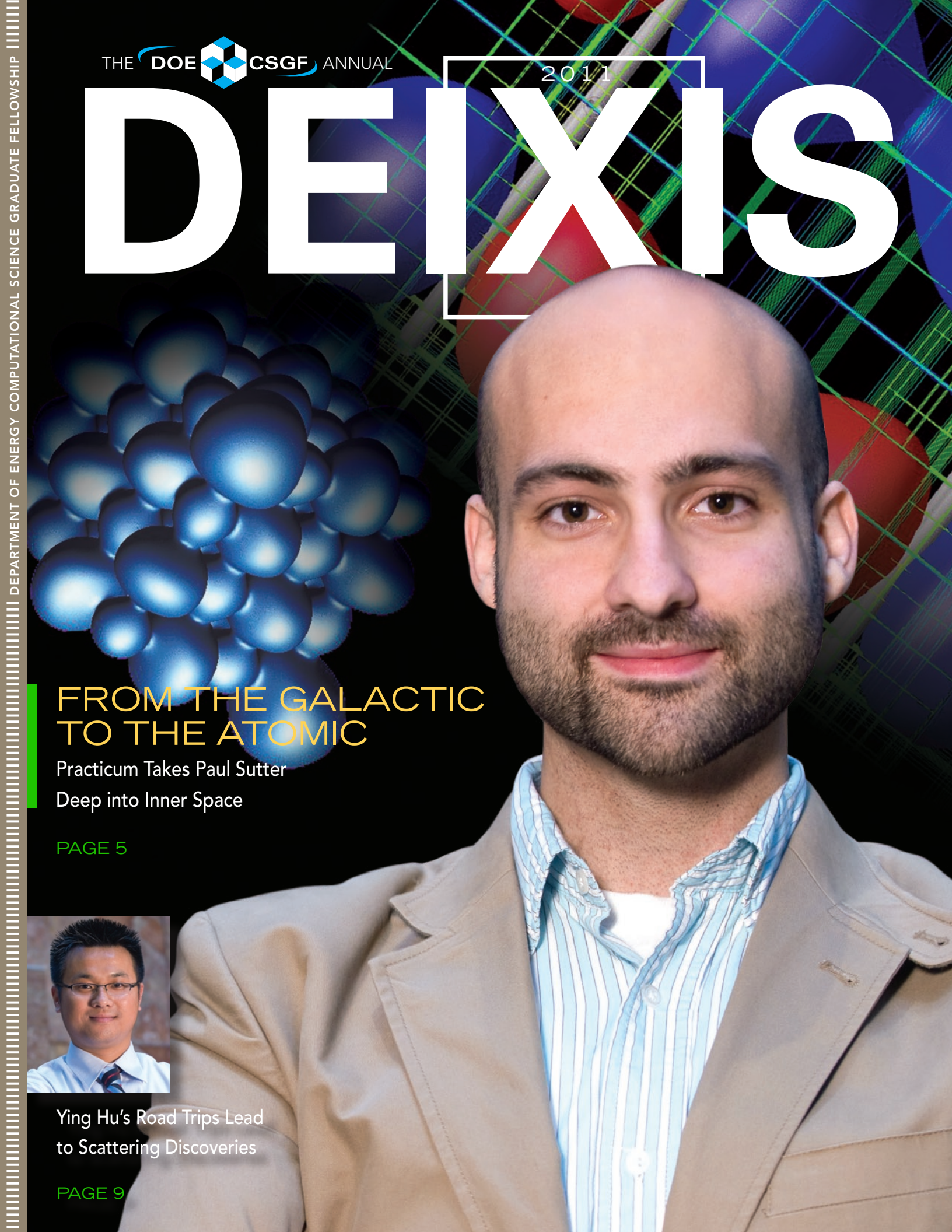
DEPARTMENT OF ENERGY COMPUTATIONAL SCIENCE GRADUATE FELLOWSHIP

THE DOE CSGF ANNUAL

DEIXIS

2011



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DEIXIS (ΔΕΙΞΙΣ — pronounced dāksis) transliterated from classical Greek into the Roman alphabet, means a display, mode or process of proof; the process of showing, proving or demonstrating. DEIXIS can also refer to the workings of an individual's keen intellect, or to the means by which such individuals, e.g. DOE CSGF fellows, are identified.

DEIXIS is an annual publication of the Department of Energy Computational Science Graduate Fellowship program that highlights the work of fellows and alumni.

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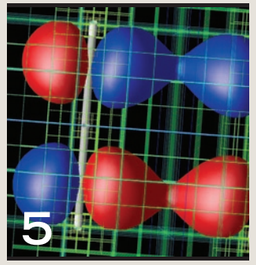

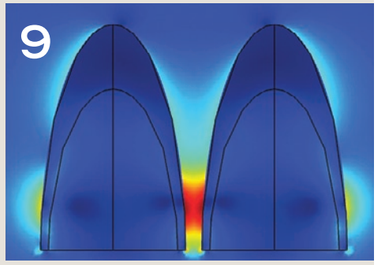

A TOAST TO 20 YEARS

20 YEARS BUILDING A COMMUNITY OF LEADERS DOE CSGF 1991-2011

In 1991, the fates of two technological tools — the Internet and computational science — became linked in the High-Performance Computing and Communications Act. The law backed creation of the "information superhighway," but also directed the Department of Energy (DOE) to support computational science education.

The Internet's phenomenal expansion is renowned, but the parallel escalation in high-performance computing for science has been equally exceptional. Since 1991, the DOE Computational Science Graduate Fellowship has led the field's maturation into the "third leg" of scientific discovery. With more than 250 alumni, it's helped create a community of computational science leaders.

This issue bears witness to the fellowship's success. Our cover story features Paul Sutter, who used his practicum to step outside his scientific comfort zone. We also announce this year's Frederick A. Howes Scholar in Computational Science: Alejandro Rodriguez, who has matched his work in computational physics with his devotion to outreach. And we feature three alumni, including Brian Moore, who found a calling in nuclear energy.

Alumni and fellows are welcome to participate in the program's essay contest, which provides them the chance to convey their research to a broader, non-technical audience. The winner, fellow Kenley Pelzer, connects onions to quantum mechanics.

Here's to 20 years — and many more to come.

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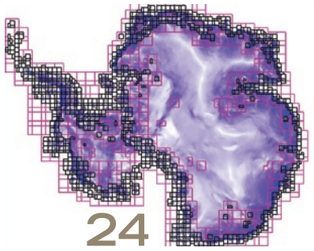

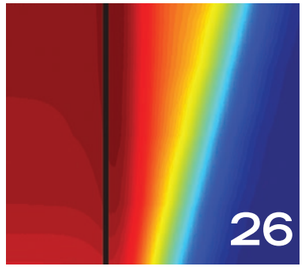

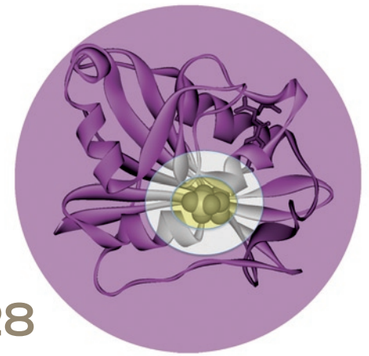

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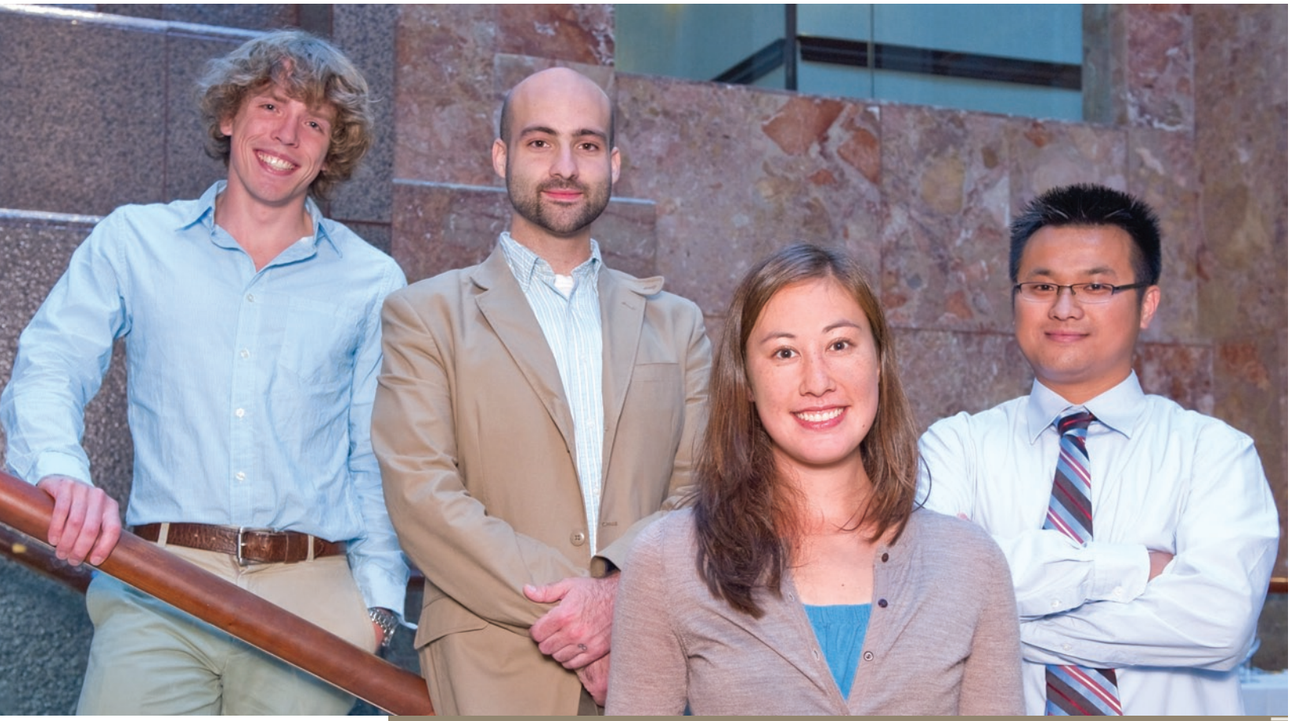
A SEASON OF DISCOVERY

FOR FELLOWS, THE SUMMER PRACTICUM NURTURES PROFESSIONAL AND PERSONAL GROWTH



Left to right:
Scott Clark, Paul Sutter, Anne Warlaumont and Ying Hu in Washington, D.C., at the DOE CSGF Annual Conference.

SUMMER PLANS often take more thought for recipients of the Department of Energy Computational Science Graduate Fellowship than for other graduate students.

Summer usually is when fellows head to DOE national laboratories to complete their required practicums. Often, they've met the scientist they'll work with at a conference or through a mutual acquaintance. But some fellows — like Ying Hu, who is profiled here — also visit several labs before choosing one.

Practicums push fellows to explore subjects or test skills with little or no connection to their doctoral research. It frequently leads them to refine a computer science skill — as fellow Paul Sutter did — or, like fellow Anne Warlaumont, to develop a greater appreciation for hands-on lab work.

Some fellows even end the summer determined to take on entirely new research subjects. Fellow Scott Clark, for instance, headed to his practicum planning to focus his dissertation on computational fluid dynamics. By summer's end, he'd found a new love: metagenomics.

That's the power of the practicum: reinvigorating, redirecting and remarkable.

The Department of Energy Computational Science Graduate Fellowship supports the nation's brightest science and engineering students, allowing them to concentrate on learning and research. The work of more than 250 DOE CSGF alumni has helped the United States remain competitive in a global economy.

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FELLOW SPANS SCALES FROM THE UNIVERSAL TO THE ATOMIC

PAUL SUTTER
University of Illinois at Urbana-Champaign
Oak Ridge National Laboratory

WHEN IT CAME TIME to choose a practicum for summer 2009, Paul Sutter went from the enormous to the minuscule.

Sutter, a Department of Energy Computational Science Graduate Fellowship recipient, usually simulated galaxy clusters, the largest structures in the universe. At Oak Ridge National Laboratory (ORNL), he calculated electronic structure in atoms.

"The energy scales, the spatial scales, the time scales are the complete opposite end of the spectrum from what I usually do," says Sutter, who earned his doctoral degree in astrophysics from the University of Illinois at Urbana-Champaign (UIUC) this spring. "And the architecture of the computer code was completely different."

It's just what he wanted. Practicums let fellows try research in areas largely outside their studies, but few go as far afield as Sutter did. "I realized that there aren't a lot of opportunities in your research career to go off and do something completely different," he says, and he took advantage of it. After meeting several ORNL researchers Sutter opted to work with Robert Harrison, leader of the Computational Chemical Sciences Group.

Sutter focused on MADNESS (Multiresolution Adaptive Numerical Environment for Scientific Simulation), a code that solves the electronic structures of atoms, molecules and nanoscale systems. Harrison led creation of the program, which is used in computational chemistry, superconductor modeling and other areas.

Calculating electronic structure is so difficult scientists must limit their models' accuracy and the size of the systems they compute. Using MADNESS, researchers can compute the properties of larger systems with higher accuracy than traditional quantum chemistry codes allow. It divides the physical domain being modeled into parts for calculation on parallel processing computers, while repeatedly subdividing the most interesting pieces for more precision.

As the program subdivides the domain it generates an "octree" structure of branching nodes. The number of nodes depends on the level of detail researchers want, the problem size and the computer they use. Typical MADNESS problems involve octrees with 10,000 to 100 million nodes.
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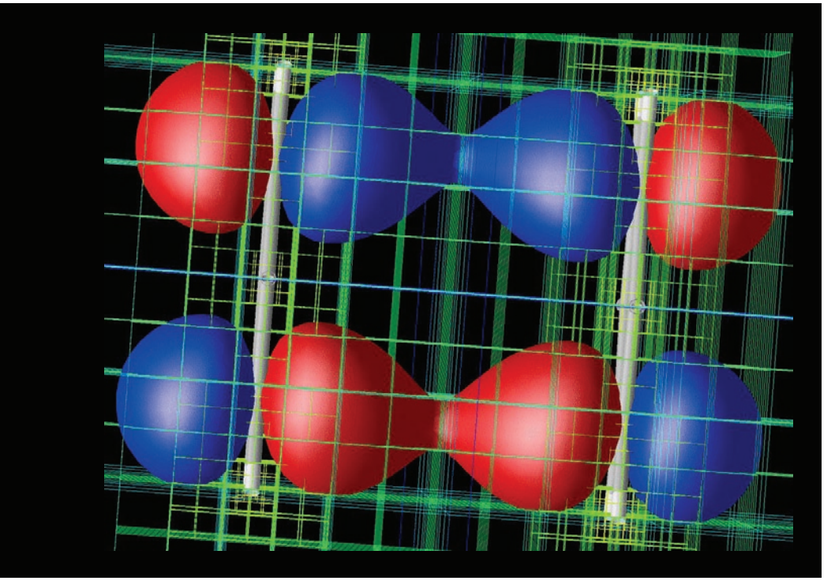

This visualization shows a molecular orbital of the benzene dimer computed using MADNESS. It shows the adaptive "grids" used to focus computation on the most important areas.

Image courtesy of Robert Harrison, Oak Ridge National Laboratory, with support from the Scientific Discovery through Advanced Computing program.

The structure makes scaling MADNESS a challenge; running it on larger computers doesn't lead to proportionately faster and more efficient performance. Some nodes require lots of work, while others require little, but there's no way of knowing which is which, so MADNESS randomly assigns them to processors.

"It results in a lot of communication, because if you want to find out what's going on with your neighbor on the tree, you know your neighbor's not going to be on your processor. It's going to be somewhere else," ORNL Computational Scientist Rebecca Hartman-Baker says. The sometimes-uneven distribution of work and the constant communication slow things down.

What was needed, Sutter says, was "some way of balancing them out. Instead of, say, 10 nodes on all processors, maybe some processors have just one node, but computationally it's a very expensive node. Other processors might then have 100 nodes, but they would be very, very cheap. So in the end the amount of work per processor stays the same."

Sutter and Hartman-Baker implemented a "melding" algorithm that splits up nodes so each processor has roughly the same amount of communication and work. But "we didn't really have a way of figuring out how much time was required on each node" to weight them for redistribution, Hartman-Baker says.

Sutter addressed that problem with a "profiling" algorithm. In effect, MADNESS runs with the random load-balancing algorithm and gathers data on how long nodes take to compute. Then it uses that data to rebalance the load on the fly. Overloaded processors send work to others while underutilized processors gather data to work on.

"Melding with profiling tries to balance the two — to only move work to another processor if it makes sense for both computation and communication," Sutter says.

Sutter ran two tests comparing MADNESS with and without the load-balancing algorithm. The first compared basic mathematical operations — multiply two functions, copy one function into another and "compress," in which MADNESS devolves a function into its constituents.

Using ORNL's Jaguar, a Cray XT5 rated one of the world's fastest computers, Sutter averaged the cost of compress, multiply and copy operations across five runs on two problems — one with about 10,000 nodes and one with about a million. The smaller problem produced little difference on compress and multiply operations but improved scaling for copy. The results were essentially the same for the larger problem — except that computing times for copy operations improved dramatically as the number of processors increased. "That was good, because copies happen a lot," Sutter says.

The second test used a real-world problem: solving the Poisson equation to calculate the electrostatic potential of a large molecule-like structure. "This problem can get very, very big very, very quickly," Sutter says. "There is a nasty list of things that have to be done."

Again, Sutter tested the algorithm on large and small problems and averaged results over five runs. Profiling and melding produced a modest gain on the large problem, cutting calculation time by almost 10 percent when compared to the standard approach. Calculation time changed little for both even as the number of processors increased.

Results were more significant for the smaller problem. Calculation time for the standard approach held steady at a bit more than 150 seconds. With the load-balancing algorithm, calculation time held steady at around 60 seconds — a 60 percent cut. "Overall, we found a pretty solid performance boost when doing this improved load balancing," Sutter says.

Working with MADNESS gave Sutter insights into extending FLASH, a multiphysics, multiscale code he used in his dissertation research. In fact, he returned to Oak Ridge last fall to work with Hartman-Baker on improving FLASH.

Sutter also got the chance to work with Jaguar, even getting the machine almost all to himself as MADNESS ran during testing after an upgrade. He and his UIUC doctoral advisor, Paul Ricker, also got an allocation on Jaguar. "It's just a dream to use," Sutter adds.

Sutter's research focused on magnetic fields within clusters of hundreds or thousands of galaxies. Astrophysicists think supermassive black holes found in a galaxy at the clusters' center may generate the fields.

The fields are weak, Ricker says — perhaps a fraction of Earth's, but spread over a large enough area that they force accelerated particles like electrons to move in a spiral-like pattern, generating radiation in the radio spectrum. Two clusters may look similar in the optical or X-ray spectra, Sutter says, but not in the radio spectrum. "Since radio is nonthermal emission we actually get signatures of the cluster's history, such as past collisions" with another cluster.

Sutter and Hartman-Baker implemented a "melding" algorithm that splits up nodes so each processor has roughly the same amount of communication and work.

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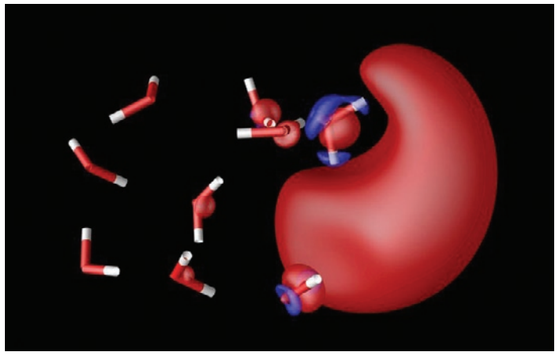

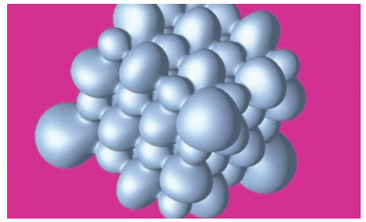

Above: MADNESS has applications in solid-state physics, including calculating the Coloumb potential for electrostatic interaction, as shown here for lithium fluoride.

Left: MADNESS can apply the Hartree-Fock and Density Functional Theory methods to calculate the ground state energies of atoms, molecules and nanoscale systems. This visualization shows a MADNESS calculation of the spin density of a solvated electron.

Images courtesy of Robert Harrison, Oak Ridge National Laboratory, with support from the Scientific Discovery through Advanced Computing program.
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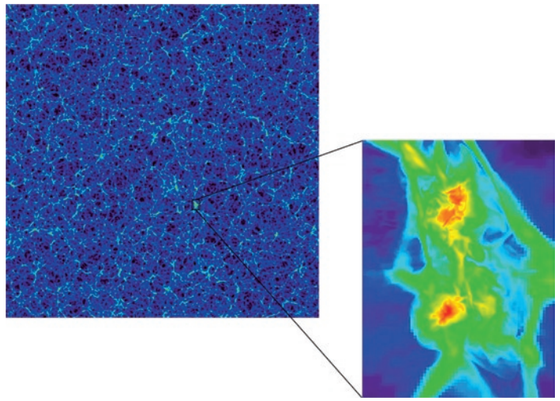

This simulation shows the distribution of gas in a section of the universe 5 billion light-years wide. The enlarged portion zooms in on a pair of merging galaxy clusters. The simulation uses adaptive mesh refinement to focus calculations on areas of interest: the central red turbulent region of the clusters, where peak resolution is a computational cell about the width of the Milky Way galaxy.

Astronomers and cosmologists are building radio telescope arrays to capture signals the clusters emit. The simulations give them ideas of the number and strength of objects they'll see. And when researchers get radio emissions data, simulations will help interpret them into a history of the cluster.

Those simulations must cover enormous swaths of space, but with enough detail to capture the injection of magnetic fields emanating from black holes. "It just becomes a very, very large problem," Sutter adds.

In one project he, Ricker and graduate student Hsiang-Yi Yang used FLASH to create simulated radio astronomy maps. They computationally evolved galaxy clusters and their radio halos over a span of 12 billion years in a "box" of space 366 megaparsecs on a side. (One megaparsec, or million parsecs, equals about 3 million light years.) The simulation had to include the influence of invisible dark matter that makes up the bulk of the universe and then calculate the movement and behavior of hot gas. Yet, it's still only precise enough to estimate just the magnetic fields, rather than radio emissions directly.

Observations show only a small percentage of lower-mass clusters has detectable halos, Ricker says, while about a third of higher-mass clusters do. Yet, the simulated radio maps predicted more low-mass, low-power radio halos and too few high-mass, high-power halos. That may result from assumptions made in the simulation, Ricker says.

Ricker and Sutter later ran a version simulating a volume of space 1.5 gigaparsecs (1.5 billion parsecs) on a side. The simulation identified the most massive clusters and the researchers used adaptive mesh refinement to focus calculations, "zooming in" on those and a large number of less massive halos. At its finest resolution, one cell in the computational data mesh was about the size of the Milky Way galaxy.

Sutter and Ricker plan to compare simulation results with actual radio telescope observations. Sutter adds, "Hopefully we can match what they see and that will give us some confidence that we're moving in the right direction."

He's fascinated by the idea that every plot, simulation or visualization he does is an attempt to portray an unimaginably enormous reality. "It's a pretty crazy idea. When I actually sit down and think about, outside of the simulations I'm doing, what this means in the real universe — it boggles my mind sometimes."

Sutter finished his doctorate while living the last two years in Newark, Ohio, five hours from Urbana-Champaign. Ricker approved the arrangement so Sutter's new wife, Mandi, could stay at her job.

"With just about any other student, I would have said this is really a bad idea," he says, but Sutter is "disciplined enough that he's been able to get an awful lot done."

That long-distance relationship is nothing compared with Sutter's postdoctoral research post. He's studying the cosmic microwave background and helping design the next generation of cosmic probes with Ben Wandelt, a former UIUC faculty member now at the Paris Institute of Astrophysics. Sutter will spend a few weeks each year in Paris, but most of the time he'll be in Ohio, working with Ohio State University Astronomy Professor David Weinberg.

What's a few thousand miles when you're discussing objects billions of light years across?

Sutter is fascinated by the idea that every plot, simulation or visualization he does is an attempt to portray an unimaginably enormous reality.

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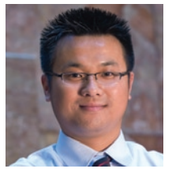
ILLUMINATING A PATH TO CANCER CELLS

YING HU
Rice University
Lawrence Berkeley National Laboratory



YING HU SWEARS HIS DECISION to pursue a practicum in California had nothing to do with the snowstorm that trapped him in his hotel during a January 2009 visit to Argonne National Laboratory near Chicago.

Hu, a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient, also visited Lawrence Livermore (LLNL) and Lawrence Berkeley (LBNL) national laboratories in the San Francisco area as he researched practicum locations.

"All the groups I visited are fabulous," says Hu, a doctoral candidate in biomedical engineering at Rice University in sunny Houston, Texas. He learned how different labs operate and discussed shared scientific interests with researchers, including LBNL's Jim Schuck and Jeff Neaton. Schuck studies nanoscale optical imaging spectroscopy, investigating how structures hundreds of times smaller than human hairs interact with light. Neaton works on the theory side, understanding nanoscale phenomena and guiding experimental researchers like Schuck.

Their work meshed well with Hu's doctoral project: Developing computer codes to investigate optical properties of nanostructures and optimize their designs — specifically to target cancer cells. And LBNL had the Molecular Foundry, a nearly new facility where nanoscale theory, fabrication, testing and simulation research share space in a dramatic building overlooking the bay area.

"It played a major role in my decision," Hu says. "It's a very integrated facility. You can fabricate a sample in the clean room and then take it to the first floor and do measurements. At the same time people on the third floor are doing calculations" to understand the results.

Hu did all three while researching surface-enhanced Raman (RAH-mon) scattering (SERS), in which scientists decipher the molecular and crystal structures of even miniscule amounts of materials by analyzing the way they react to light.

"You excite the molecule at one wavelength and you collect the whole spectrum and look for the Raman peaks," Hu says. Like fingerprints, "The locations of the peaks are unique to each molecule." The effect is weak, but in the 1970s researchers found that placing samples on roughened metal surfaces significantly boosts scattering — thus the SERS name.

Scientists have postulated two explanations for the SERS effect, one arising from chemical bonds between the material and the metal surface, and one from electromagnetic interactions. Hu explored each.

Both projects focused on a substrate of nanocones made of silicon-germanium and coated with a thin layer of gold. It's like a field packed with a jumble of irregularly sized gold-plated traffic cones, each a thousand times thinner than a hair.

"What we're proposing is that by just using one added step you can improve the sensitivity and probably detect something you couldn't detect before," Hu says.

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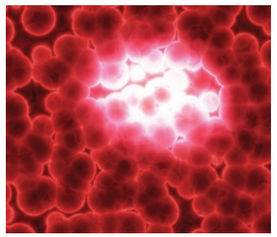


REWARDING REQUIREMENT

All DOE CSGF recipients must complete a practicum at a national laboratory by the end of their second year — a requirement Ying Hu found a bit intimidating.

"In the beginning you feel like, 'OK, it just adds another three months that I need for graduate school. It delays my graduation date,'" says Hu, who earned his doctorate at Rice University earlier this year.

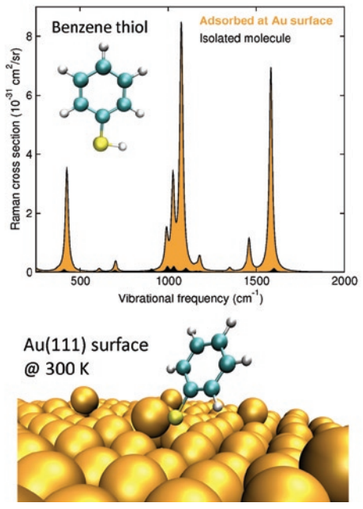
He changed his mind after doing research at Lawrence Berkeley National Laboratory in summer 2009. The experience, Hu says, expanded his horizons. He learned how another lab in an area similar to his doctoral research operates, what computing and experimental resources are available in the field, and what other researchers are thinking.

Hu's summer in Berkeley — and a second practicum at Lawrence Livermore National Laboratory in fall 2010 — also allowed him to begin building a network of colleagues and possible collaborators.

"It's really a start for me to think about my career path, to develop my own perspective on what I think should be done or can be done (in his field) in a more realistic way," Hu adds. "It's something that's hard to get from staying in the lab in graduate school."

During his practicum, Hu studied how the way that a benzene thiol (BT) molecule binds to the substrate — like how a Tinkertoy stick-and-ball model might fit in a socket on the gold traffic cones — affects SERS. The researchers computed relative Raman scattering enhancement for each of three binding configurations and compared the results with actual SERS measurements.

The researchers chose BT because it's relatively simple to compute. "But it by no means is an easy molecule to work with"



The graph shows Raman cross sections of benzene thiol with the isolated molecule tracked in black and the molecule chemisorbed on a Au(111) surface in orange. Chemical enhancement leads to the much stronger intensity from the chemisorbed molecule. The image below the graphic simulates the binding geometry of benzene thiol on a Au(111) surface at 300 K. This shows that at room temperature the binding geometry of benzene thiol on Au(111) is not well defined, both with respect to molecular orientation and sulfur-gold bonding coordination. Sulfur typically tends to pull one gold atom from the surface.

experimentally, says Hu, who prepared and scanned the samples. "It's a very potent chemical and it has a very strong, skunk-like odor."

ENHANCED UNDERSTANDING OF ENHANCEMENT

They found the way light perturbs the charge transfer complex between BT and the gold atoms affects SERS. To continue the analogy, how much scattering is enhanced relies on how light affects the connection between the Tinkertoy and gold on the traffic cones. Some configurations yielded a stronger response than others. In some cases, computer calculations agreed with the experimental results.

Hu presented the research in a paper coauthored with Schuck, Neaton, and LBNL and University of California, Berkeley researchers Alexey Zayak, Hyuck Choo and Stefano Cabrini. "It's a relatively new theory to explain chemical enhancement," Hu says. "I think it's going to have a relatively big impact."

Schuck says that while different mechanisms for enhancement have been proposed over the past 30 years, no one knew which were important until Hu and his fellow researchers came along. With the interpretation in the paper, "For the first time, we have a general quantitative basis for understanding chemical enhancement for all SERS measurements, which I think is pretty amazing."

Hu tackled SERS's electromagnetic foundation after returning to Rice and discussing ideas with Seunghyun Lee, a chemistry graduate student. Other collaborators include Berkeley Lab's Choo; Jaeseok Jeon and Tae Seok of UC Berkeley; Hu's advisor, Rebekah Drezek; and Lee's advisor, Jason Hafner.

Electromagnetic enhancement of SERS is believed to arise from surface-plasmon resonance — the nanostructures' response to electromagnetic radiation. In essence, the gold nanocones act like tiny antennae. Their electrons oscillate in response to visible light because the structures are similar in size to the light's wavelength — 400 to 800 nanometers.

In a typical SERS setup, a laser hits the molecules to be tested — located on the metal substrate — from directly above, Hu says. "Most of the time, if you think of light as electromagnetic waves, the polarization can only be perpendicular to the direction it's propagating," he adds. A laser coming directly from above will be polarized in the transverse plane — horizontal to the surface. It can't be axially polarized — perpendicular to the substrate.

But the researchers' simulation showed axial polarization would generate stronger electromagnetic enhancement in the nanocones. "So that creates problems," Hu says. The researchers tackled them by spreading gold nanoparticles on the substrate — like dropping gold balls on the field of traffic cones. Tests found nestling the nanoparticles between the cones boosted SERS activity by more than a factor of 10, even with transversely polarized light, Hu says. Experiments bore out the results, which are reported in a paper accepted for publication in the journal *ACS Nano*.

"What we're proposing is that by just using one added step you can improve the sensitivity and probably detect something you couldn't detect before," Hu says. Fine-tuning nanoparticle size and concentration could enhance scattering even more, he adds.

While at LBNL Hu also adapted MEEP, an electromagnetic physics code, to run on parallel processing machines at the Molecular Foundry. The task required installing and coordinating multiple software packages. "That was really a learning experience for me because my background is not computer science," Hu says.

Hu arrived at LBNL, Schuck says, just as he and Neaton "realized there was a whole new range of things we could do that needed to go parallel." Since Hu installed MEEP, "we use it a ton."

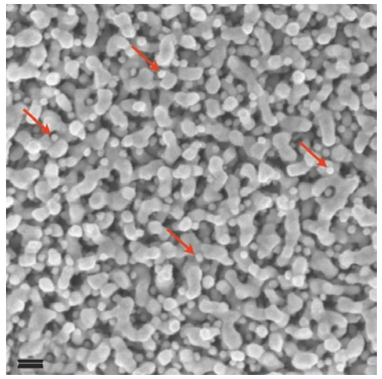
TINY TIES

Hu used MEEP to simulate the nanoplasmonic response of bow-tie antennae — tiny gold triangles pointing to each other. In Hu's calculations, there were four triangles, arranged like a Maltese cross, on a dielectric substrate. He studied the consequences of moving a triangle off center.

"By shifting one element we can actually concentrate light at different locations in the structure at different wavelengths," Hu says, and different configurations can sort light of different wavelengths.

The color-sorting antennae could be used in optical computers, which transmit information with photons instead of tiny wires printed on silicon chips, Schuck says. But a more near-term application may be in extremely small and fast multicolor light detection for cameras and sensors.

LBNL researchers were still analyzing Hu's data and producing papers based on it more than a year after he finished his practicum, Schuck says. "We can't help but send Ying e-mails and ask him questions, because we know he knows the answers to a lot of these things. We'd love nothing more than to work with Ying" again.



This scanning electron microscope image shows an overhead view of the nanocone substrate for SERS, seeded with gold nanoparticles (red arrows) to test how seeding enhances Raman scattering. Scale bar (lower left) is 100 nanometers.

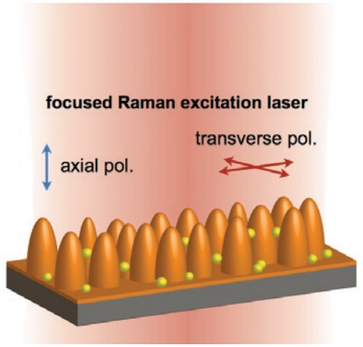
Hu was familiar with calculating nanoplasmonic effects. His doctoral research focused on nanoshells: minuscule hollow or layered gold balls. In Drezek's lab, researchers conjugate the particles with antibodies that target cancer cells. Once injected into the body, the nanoshells attach to tumors.

By adjusting their size and geometry, researchers can "tune" nanoshells to absorb or scatter specific light wavelengths. The Rice team engineers nanoshells to resonate with near-infrared light, a spectrum minimally absorbed by surrounding tissue. When a near-infrared laser shines on the particles, they illuminate, defining the tumor's edges.

The surface temperature of the nanoshells also rises quickly as they absorb light. By increasing the laser's power it may be possible to "cook" and kill cancer cells with minimal harm to healthy tissues.

Just a few years ago most nanoshell designs were simple enough that standard computers usually were enough to calculate their properties, Drezek says. Now the nanoparticles labs produce are so complicated it takes parallel processing on a cluster to understand them.

"We weren't doing any of that in our lab before Ying started. We just did our simulations on desktop computers," she says. "He was able to take all the computational coursework, move what he was doing into the clusters and open up all sorts of different opportunities for us."



This illustration shows axial and transverse (in-plane) polarizations (in relation to the SERS substrate) of laser light for Raman excitation. Research by Ying Hu and colleagues suggests that seeding the surface with gold nanoparticles, as shown, boosts SERS activity by more than a factor of 10 with transversely polarized light.

"We weren't doing any of that in our lab before Ying started. We just did our simulations on desktop computers," Drezek says. "He was able to take all the computational coursework, move what he was doing into the clusters and open up all sorts of different opportunities for us."

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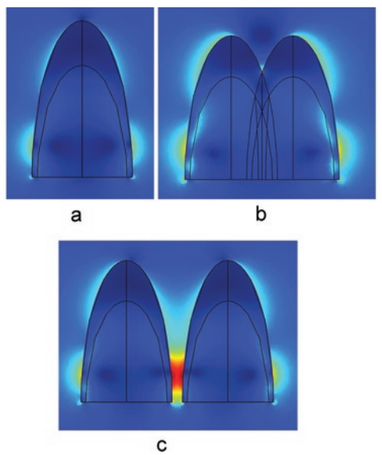
In a paper published in the Nov. 24, 2008 issue of the journal *Optics Express,* Hu, Drezek and Rice biochemistry student Ryan Fleming simulated a nanoshell comprised of a gold outer layer, a silicon inner layer and a gold core. The calculations found each layer's plasmonic resonance mode interacts with the others. "That interaction is what renders these particles tunable, like how we can tune it to the near infrared spectrum," Hu says.

Hu graduated this summer, just nine years after moving from China to Houston, where his parents are researchers at the Baylor College of Medicine. His mother's father, a physics professor, inspired Hu's interest in science. He recalls his grandfather floating a magnetized needle on a piece of tissue paper. The wet paper sank, leaving the needle pointing north on the surface. "It was the first compass I'd ever seen and I have to say it is the coolest compass I've ever seen," Hu says.

Hu's dissertation includes a chapter on his LBNL work and he's still collaborating with scientists he met there. "It's just another proof of the value of the practicum," he says. "It's really the start of my own independent research."

In fact, Hu did another practicum at LLNL in fall 2010, with electromagnetics and photonics researchers Daniel White and Tiziana Bond. "I talked to them during my practicum-hunting trip," he adds. "I just decided to do a second one because I liked the first so much."

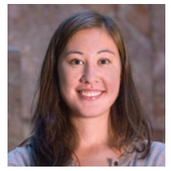


These computer simulations of gold-coated nanoscale cones show how spacing affects electromagnetic enhancement for surface-enhanced Raman scattering.

A single cone (a) or a doublet (b) does not exhibit strong enhancement under transversely polarized light, while a narrow gap between two nanocones (c) does.

MODELING A NEURAL NETWORK

ANNE WARLAUMONT
University of Memphis
Argonne National Laboratory



Warlaumont says the project gave her a different perspective. "In my main research I build neural network models. Those models are even more abstract than the ones we worked with (at ANL). I was happy about the opportunity to work with a detailed model and see what I was missing."

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USUALLY, ANNE WARLAUMONT DEALS only with the rough computer counterpart to a brain — building "neural" networks that classify sounds from babies and emulate the way they learn to speak.

But Warlaumont, a Department of Energy Computational Science Graduate Fellowship recipient, saw the real thing during her summer 2009 practicum at Argonne National Laboratory (ANL) near Chicago.

Warlaumont shadowed two students in University of Chicago (UC) researcher Wim van Drongelen's lab and witnessed electrophysiology experiments on mouse and human brain tissue. As her practicum ended she also watched brain surgeons operate on a girl who suffered epileptic seizures since infancy.

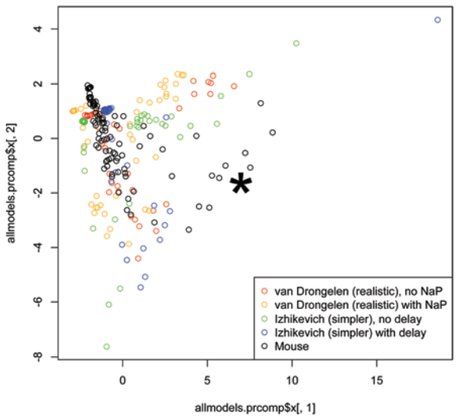
"I definitely never thought I would see something like that. It was a special bonus," says Warlaumont, a doctoral student in the School of Audiology and Speech-Language Pathology at the University of Memphis (UM).

Warlaumont's peek inside the skull was only appropriate. In her practicum, she designed a program that compared detailed and abstract computational models of an epileptic brain. While working with Mark Hereld, an ANL experimental systems engineer in the Mathematics and Computer Science Division; ANL Associate Laboratory Director for Computing, Environment and Life Sciences, Rick Stevens; and van Drongelen, Hyong Lee and Marc Benayoun at UC, she also compared the models with activity recorded from slices of mouse brain tissue.

Warlaumont says the project gave her a different perspective. "In my main research I build neural network models. Those models are even more abstract than the ones we worked with (at ANL). I was happy about the opportunity to work with a detailed model and see what I was missing."

The models Warlaumont develops in her UM research "learn" to identify infant utterances — the vowels, squeals, growls, grunts, babbling, crying and laughing babies do as they test their speech abilities and learn to talk.

"There are theories of how infants develop the ability to vocalize and theories of how infants learn sound and why they produce some sounds before others," she adds. "There is a small group of us interested in translating some of the theories into a way to more rigorously test those computationally." The end results could include better speech analysis tools or even a model that perceives sounds — both from others and from itself — and learns to "speak" much as infants do.



Each colored point in this figure represents a single neural network model run's behavior, plotted in an abstract 2-dimensional "behavior space." Red and orange points are from the two versions of the detailed model; green and blue are from the two versions of the abstract model. Each run within a model version has a different combination of excitation- and inhibition-related parameters. Black points and the star represent samples from a recording of real mouse brain tissue.

"I have several different research threads, all related to infant vocalization research and understanding the computational or technological components involved," Warlaumont says. "I see these as part of a very long-term research program."

Warlaumont and Hereld hope her practicum project will help us better understand brain activity by improving neural models, which range from highly complex and computationally demanding to abstract and easy to run.

"Our project was comparing temporal signatures of neural network data produced by a couple of very different types of computational models. We wanted to compare them with each other and with a real system of brain cells," Warlaumont says.

For example, the researchers wanted to know whether the advantages of a highly realistic model outweigh the demand it places on computer resources. "This project is helping us to understand how low can we go — how simple and therefore computationally fast we can make a model that will still deliver appropriate results," Hereld says.

Warlaumont adds, "Another factor is your ability to understand what's going on with a model. The more detailed a model is, the more like a real system it is, but it may be so complex it's hard to understand." On the other hand, simpler models aren't as readily tweaked to match reality.

The researchers had their work cut out for them. "The problem is pretty difficult because it's terra incognita," Hereld says. Scientists typically have some intuition about the relevant processes behind a phenomenon, but epilepsy's complex, variable nature resists prediction.

The researchers ran two models, one detailed and one abstract, then compared average cell membrane potential — a measure of the voltage difference between the interior and exterior of a cell. Neurons use electrical membrane potentials to transmit signals between different parts of the cell and to initiate communication across cells.

Van Drongelen designed the detailed model, which simulated 656 neurons of six different kinds. Each cell is modeled as a set of compartments corresponding to its parts and includes chemical channels that regulate spontaneous firing and transmission of nerve impulses between cells.

The researchers ran two versions: One with persistent sodium ion channels and one without. Persistent channels could be important to understanding network behavior, Hereld says.

IN THE ABSTRACT

The more abstract model, developed in 2003 by Eugene Izhikevich, then of the Neurosciences Institute in La Jolla, Calif., treats each neuron as a single compartment and randomly varies parameters to model different types. Neurons are networked more randomly and a simpler mathematical method models ion channels.

The researchers also ran two versions of this simpler model: one with instantaneous transmissions between neurons and one with a six-millisecond delay. They compared simulation results with data recorded from slices of mouse frontal lobe tissue that was excited to produce normal and seizure behavior.

The detailed simulations ran on Jazz, ANL's recently replaced 350-node computing cluster. Each persistent sodium version took about 200 seconds to run. In contrast, each run of the abstract model's instantaneous transmission version took about 10 seconds on a standard laptop.

For each model and for the mouse data the researchers averaged neuron activity across all the cells. That was tricky: Both models generated data in physical units — microvolt waveforms — but they had different temporal resolutions and some unimportant differences. Those disparities are "one of the reasons we had to struggle to try and eliminate artifacts and find real differences," Warlaumont says.

The researchers filtered simulation results to make them comparable to mouse brain traces, then extracted eight primary metrics from each time series. "We looked at things like, within the network, are all the neurons spiking? If there is a lot of heavy synchrony in the firing of neurons, it would end up leaving traces of big peaks and valleys in the network signal," a sign of a possible seizure, Warlaumont says. "We also looked at the spectral character of those network voltage signals, the amount of power in different frequency bands."

They ran a principal components analysis to reduce the dimensionality of the behavioral features space. That let the researchers compare the range of behaviors a given model produced.

Ultimately, the abstract models seemed to produce a range of behaviors as broad and nearly as similar to mouse data as the detailed ones. "You are not necessarily disadvantaged, from that perspective, if you use the less detailed version," Warlaumont says. Yet, "I wouldn't want to make it sound like simple models are always better, because there are advantages to detailed models."

As to what this work means for understanding and treating epilepsy, Warlaumont says computational models of brain disorders are imperfect, but still informative and can help guide research.

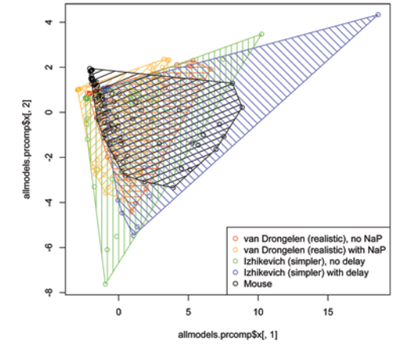
"Assuming you accept that computational modeling is valuable for those purposes, it's a logical next step to ask how we are going to objectively compare these models," she adds. "It's not a big problem now because there are only a few, but if you see a future for this there will be more models. I think figuring out how to compare and evaluate those is important."

GRASPING SPEECH DEVELOPMENT

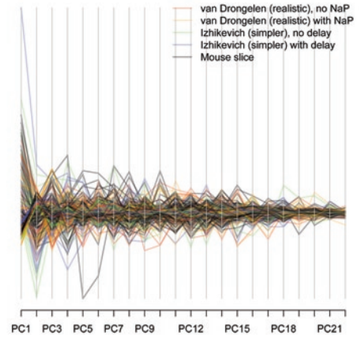
The details of speech recognition and learning Warlaumont hopes to emulate in her UM dissertation research are too complex to capture with the models and computing technologies available today. Still, she hopes her work will help researchers better understand speech development.

One of Warlaumont's models, built in collaboration with UM colleagues Eugene Buder, Robert Kozma and Rick Dale, is a neural network that recognizes protophones — early categories of infant vocalizations — with potential ramifications for speech analysis.

Currently infant speech research depends on assistants who spend days listening to recordings and manually coding each sound for its type and other properties. It's time-consuming, expensive work, and the amount of data to be sifted is growing. Coders also must make subjective judgments about how to classify a protophone, leading to inevitable inconsistencies.



Top right: The points in this plot are the same as in the page 14 plot of the detailed model, abstract model and mouse tissue in 2-D abstract "behavior space." In this figure, convex hulls are drawn around each model version's behaviors, indicating the range of behavior and the amount of overlap across the models. The abstract models produce a wider range of behaviors than the detailed models and the real mouse brain tissue.



Right: Each colored line in this plot represents one neural network model run or one sample from a mouse brain tissue recording. Different principal components (i.e., dimensions of an abstract, 22-dimensional "behavior space") are on the x-axis, and models' coordinates with respect to those principal component dimensions are on the y-axis.

"Our project was comparing temporal signatures of neural network data produced by a couple of very different types of computational models. We wanted to compare them with each other and with a real system of brain cells," Warlaumont says.

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The neural networks Warlaumont and colleagues are developing and testing automatically classify infant vocalizations, helping researchers better understand how humans perceive them and creating data that's more standardized.

Their model, reported in an April 2010 paper in the *Journal of the Acoustical Society of America*, first converts utterances into spectrograms — frequency, duration and intensity represented as 225 shaded pixels on a square. Those are sent to a type of neural network, called a self-organizing map (SOM), of 16 nodes mathematically arranged in a four-by-four grid with randomly weighted connections between each.

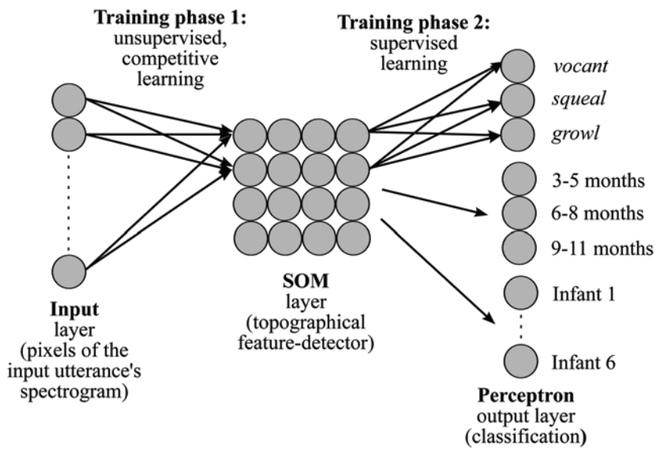
The SOM is "trained" by matching random spectrograms with the nodes whose weights are most similar to it, then updating that node's weights and its neighbor's weights. It's similar to how real brain cells develop connections based on the animal's particular previous experiences, Warlaumont says.

Each vocalization triggers states of SOM node activations, which are sent to a second layer, a neural network called a perceptron. The perceptron measures the relevance of the learned SOM features to various categories, classifies the protophone and determines which SOM nodes best distinguish one utterance from another.

After training, the perceptron can classify each protophone input by type and infant age and identity, based on SOM layer node activations. In tests, the model performed significantly better than chance. It guessed the correct protophone more than half the time, the infant's age 42.8 percent of the time, and its identity 32.4 percent of the time. "It is understandably very hard to classify age and identity on the basis of a single second of vocalization. We might be able to average many vocalizations in a recording and get better performance," Warlaumont says.

The model is a step forward, says D. Kimbrough Oller, Warlaumont's doctoral advisor. "We're testing its basic capabilities and developing the scripts and tools we need to go on to much more exact things."

Warlaumont will have lots to contribute to the effort, Oller says. She "is going to have a very significant academic career in helping to establish not only new foundations in the theory of vocal development, but the application of the tools that she's developing."



This schematic shows the neural network used to classify infant vocalizations. It combines a self-organizing map (SOM) and a single-layer perceptron. Pixels of an utterance are presented first to the SOM. Activations of SOM nodes are then sent to the perceptron output nodes for classification according to protophone, age and infant identity. The weights from the input layer to the SOM layer are trained first, then weights to the SOM are frozen and the perceptron's weights are trained.

PRACTICUM CHARTS CAREER COURSE BEYOND THE VELVET ROPE

SCOTT CLARK
Cornell University
Los Alamos National Laboratory

ONE OF SCOTT CLARK'S WEAKNESSES, if it can be called that, is that there are just too many captivating challenges.

"I've always liked to explore new and interesting things," says Clark, a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient. "One of my problems is I don't really settle on one."

That willingness to follow what fascinates him set Clark on a new course after completing his DOE CSGF practicum in summer 2009. Characteristically, he told coordinators at the national laboratories he just wanted to work in an interesting group investigating interesting problems. Aric Hagberg, coordinator at Los Alamos National Laboratory (LANL) and himself a DOE CSGF alumnus, connected Clark with Nick Hengartner, a researcher with the Information Sciences and Technology Metagenomics team.

Metagenomics approaches biotechnology in a new way. Rather than sequencing the DNA of individual microorganisms, it decodes genomes from entire communities of organisms, like in the human gut or a tidal pool. Then it compares chunks of sequence data to learn important information about the organisms' genes.

When he started his doctoral studies at Cornell University in 2008, Clark had planned to do research in computational fluid dynamics (CFD). He loves the subject, which he began studying as an undergraduate at Oregon State University, but it's a fundamental field that's been scrutinized since computers were invented. He wanted to get into an area where new things are happening and changing and "I might be able to make some big contributions right off the start."

Goodbye, CFD. Hello, DNA. After a summer working with Hengartner and Joel Berendzen in LANL's Applied Modern Physics Group, Clark made an unusual leap: from the engineering-oriented world of fluid flow to the biological realm of metagenomics.

He returned to Cornell with a new research focus. "I was hooked and I haven't looked back," Clark adds.

"It's a field where you can very quickly describe what's going on, which I really like because my friends and family can understand what's happening," Clark says, "but then getting the actual solution is much more difficult."

Metagenomics is possible thanks to rapid "shotgun" genome sequencing technology, which breaks an organism's DNA into chunks, then copies and "reads" them to record the order of the base pairs. With today's fast, relatively inexpensive sequencing scientists can read genomes multiple times for greater accuracy. The DOE supports metagenomics research as it seeks genes that can help microorganisms convert plant materials into biofuels more efficiently and cheaply.

After a summer working with Hengartner and Joel Berendzen in LANL's Applied Modern Physics Group, Clark made an unusual leap: from the engineering-oriented world of fluid flow to the biological realm of metagenomics.

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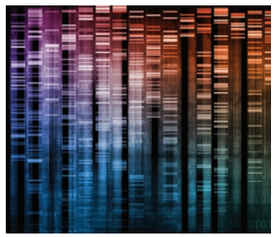
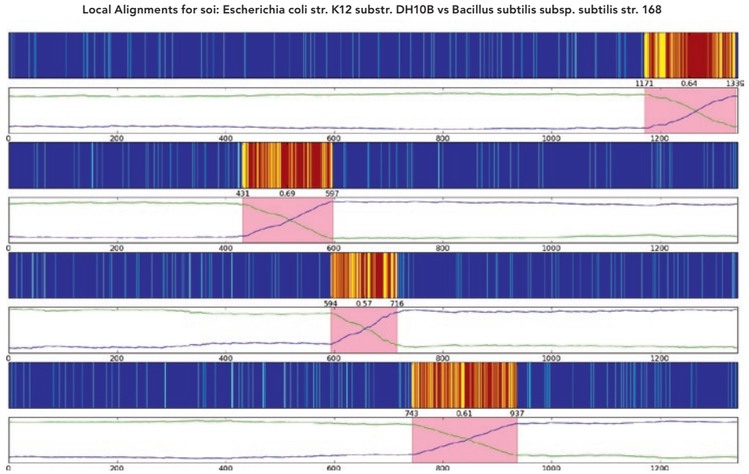


WELCOME TO THE (SEQUENCE) CLUB

Velvetrope uses two filters to find offsets — areas where two genetic sequences are more similar than expected. This visualization shows four vectors that passed a global filter test with regions marked and shaded as having possible sequence alignments. Blue means no match. Cyan marks a possible random match because it doesn't occur in the same region. Yellow marks regions of possible alignment and red marks positions in the region that have matches. The location of the region is marked along with the total density of matches within that region.



But metagenomics also produces an enormous and complex biological puzzle, as scientists reassemble and analyze billions of DNA chunks representing trillions of base pairs. Only massive computational power can do the job.

GETTING ALIENED

At LANL Clark worked on algorithms to find alignments: chunks of DNA in which a sequence of base pairs or the amino acids they code for are highly similar in the genomes of different organisms. Scientists say these sequences are "conserved" because they weren't excised through natural selection. Once researchers have multiple DNA chunks, or reads, with signatures of conserved sequence, Hengartner says, they can see how sequences align in multiple genomes "just to make sure they're all pretty much from the same place."

It's rare for large sequence chunks to be identical from genome to genome, but how similar reads align helps scientists understand the sequences' importance. "If a particular region was conserved across many different genomes, possibly in different places, it almost surely has some genetic benefit," Clark says. "You also can find relative comparisons like mutation and silent mutation rates within these conserved sequences across all genomes. That would allow us to get some information about the evolutionary distance" between two organisms.

Sequence alignment algorithms are available for parallel computers, but they demand a lot of power, Clark says. Other algorithms have difficulty dealing with transpositions — like gene A appearing before gene B in one sequence but B appearing before A in another. They try to force the two sequences together, "and invariably either give you that the As align and nothing else aligns, or the Bs align but nothing else does."

Some programs approach sequence alignment by seeking matches of a specified length, called "*k*-mers," where *k* is a specified number of base pairs or amino acids within a read. For example, the DNA read ATCGGC has the 4-mers ATCG, TCGG and CGGC within it. The program uses *k*-mer matches as "seeds" to index the genome. But "if you have a sequence that's not superconserved (completely identical) or where every third amino acid might be slightly different — statistically that's a significant conservation" worthy of study, Clark says, but some programs won't spot it.

BEHIND THE VELVETROPE

The approach Clark helped develop, named Velvetrope (see sidebar), skips finding *k*-mers in favor of seeking areas where sequences share many similarities. "It's a complex search for mostly conserved areas or statistically significant conservation, using filtering effectively and doing it in a very modular way so it can be readily parallelized," Clark says.

Velvetrope uses two filters. The global filter finds offsets — areas where two sequences share a higher-than-expected similarity. The second, local filter looks at those offsets more closely to find areas with higher-than-expected similarities within them. "Each filter is a statistical step to see whether there's a significant amount of matches," Clark adds. "You slowly refine that search until you get just the area you're interested in."

Velvetrope uses bitwise comparison to find similar offsets. A sequence of interest, with letters representing the DNA base pairs or amino acids, is lined up with a sequence from another genome. To find matching offsets, the first sequence remains stationary while the second is shifted to the right or left, one letter at a time.

"You're comparing No. 1 to No. 1. Then you shift the second sequence over one. Now you're comparing No. 1 to No. 2," Clark says. "By shifting one sequence and comparing it to a stationary sequence, you're effectively comparing all the different offsets, which allows for some really quick computational techniques."

With metagenomics producing datasets in the terabytes — millions of megabytes — speed was important to Clark, Hengartner and Berendzen. They took a computer science approach that emphasized simplicity and parallel operation. Velvetrope's modular approach makes it especially amenable to computation on general-purpose graphics processing units (GPGPUs), the chips made for video games that now are a major part of the newest supercomputers.

The Velvetrope name is meant to evoke the feeling of an exclusive club, Scott Clark says. The algorithm compares DNA or amino acid sequences to find similar sections, gradually restricting criteria to find the most relevant areas.

"The idea was it was like a nightclub and you would get deeper and deeper into it with more and more credentials," Clark says. "The barrier at a nightclub is always a velvet rope." Only sequences that match certain specifications get to the "club's" most exclusive part.

Clark and Los Alamos National Laboratory researchers Nick Hengartner and Joel Berendzen kicked around several names, like "bouncer," before Berendzen came up with "Velvetrope." They weren't concerned that another genomic tool is called Velvet because it involves genome assembly, not searching.

Ironically, since starting sequence assembly research last summer at Lawrence Berkeley National Laboratory, "I'm using Velvet all the time," Clark says.

By shifting one sequence and comparing it to a stationary sequence, you're effectively comparing all the different offsets, which allows for some really quick computational techniques.

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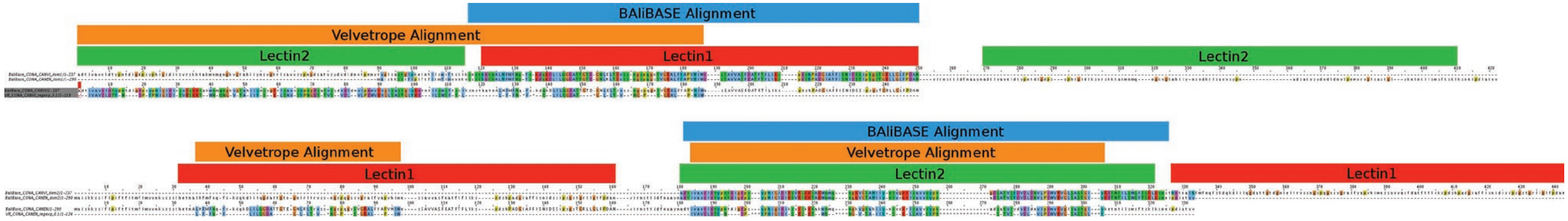
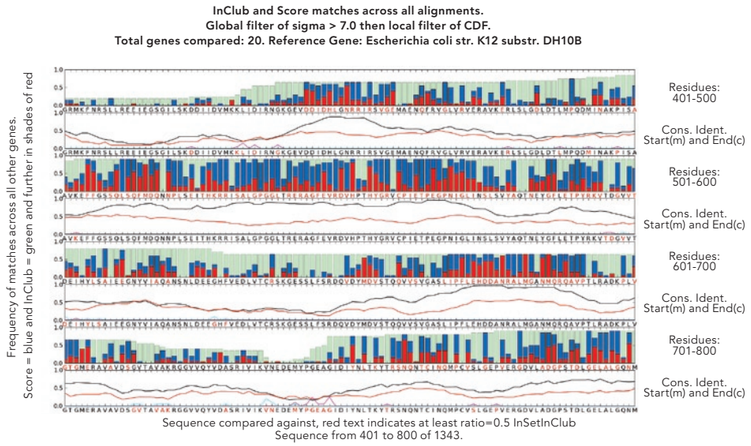


Above: This shows two sets of alignments of two Lectin protein sequence domains, with red corresponding to the Lectin1 domain and Green the Lectin2 domain. Orange is the Velvetrope alignment obtained by remapping the areas of high shared identity across the previous set to the sequence of interest. Blue is the alignment from BAliBASE, a traditional sequence alignment program. It resolves the two-domain comparison by manually specifying which domain to align (Lectin1 in the first alignment and Lectin2 in the second). This causes the aligning algorithm to append whatever domain is not specified to the beginning or end of the alignment. Velvetrope picks out homologous areas regardless of position in the sequence without specification. Lectin1 has low homologous identity in the latter part of its domain; therefore Velvetrope doesn't pick it up while the non-homology components of BAliBASE align it. It's still picked up by the Velvetrope "club" filter.



Below: Comparing a sequence of interest against a large set of test sequences lets Velvetrope find areas within that sequence that are homologous to multiple test sequences. This histogram combines information about shared identity (solid blue columns) and "club membership" (light, always larger green columns) — areas of high local homology — across many test sequences. This helps find areas of the sequence of interest that are shared among a large percentage of the whole set.

Hengartner says he and his Los Alamos colleagues pushed Clark to adapt the code for GPGPUs, stretching the fellow's abilities and enabling the program to run on desktop computers. "We're developing tools that a biologist or practitioner can use on his desktop," he adds. "This is something that is very dear to my heart — developing something that is usable by the community."

Hengartner praises Clark for achieving the goal with a minimum of direction. "It's not like there was a tremendous amount of hand-holding. I was highly impressed" with Clark's initiative.

Comparing Velvetrope's performance with other gene alignment software is difficult, Clark says. "When you compare two sequences you found in the wild, there's no answer key that says this should align perfectly or this conservation is enough." Yet, Velvetrope did find the same or similar areas of alignment as BLAST and HMMer, two gene-alignment software tools. The researchers are making Velvetrope available for free download as an open source project.

SOME ASSEMBLY REQUIRED

Clark's fascination with metagenomics led him to a second practicum in summer 2010 at Lawrence Berkeley National Laboratory (LBNL), where he worked with Zhong Wang, a researcher in the Joint Genome Institute, on a project connecting multiple DOE labs. Wang's lab emphasizes sequence assembly — using computers to put DNA reads in the correct order. One of the algorithms Clark worked on uses sequence reads early in the process, rather than toward the end as is traditionally done, to accelerate assembly. The approach also helps make the calculations easy to run on parallel computers.

At LBNL Clark also worked on a machine-learning algorithm that scores a sequence assembly's accuracy based on the data it generates. Current assembly scoring metrics are loose and somewhat arbitrary, Clark says. The approach he and Wang are developing builds formal likelihood models of an assembly given the reads already available. That lets researchers find the probability of a given assembly and use it to validate the assembly or suggest changes to improve the score.

Peter Frazier, Clark's doctoral advisor and an assistant professor in Cornell's School of Operations Research and Information Engineering, is collaborating with Clark, Wang and LBNL's Rob Egan on a paper describing the scoring algorithm. Next they want to optimize it to improve the quality of an assembly, Frazier says, with an ultimate goal of applying the algorithm to metagenomic assembly.

Clark and Frazier also are working with researchers from Cornell's College of Veterinary Medicine and Department of Computer Science on genomic approaches to find bacteriophages — viruses that infect bacteria — able to treat *Escherichia coli*-related ailments in cows. The researchers hope to find useful features in the phages' genomes, then use machine learning, optimization and experimental design to mix the best viruses in a "cocktail" for bovine infections.

With his unusual combination of expertise in computation, mathematics and biology, "Scott's been playing more of an advisory role," to bridge the gap between the two research communities, Frazier says. "We'd be talking with biologists and … sometimes it would be sort of hard to have each of us understand what the other one meant." Clark "was very valuable from that point of view — and then he's also just wicked in terms of computation."

Clark is one of the few people who could tie a career in computers to cows. The Oregon native started programming at age 8, "much to the chagrin of my parents, who were both journalism majors." He played with PCs from garage sales, and in high school launched a Web page design business. At Oregon State he started in mathematics and computer science but switched to math and physics. While still a freshman, he talked his way into a graduate-level computational physics course with legendary professor Rubin Landau, who later became his mentor. "From that day on I was in love with computational science," says Clark, who earned bachelor's degrees in mathematics, physics and computational physics.

In the long run, Clark sees himself starting a biotech or computational science business. His lab experience, however, also has him considering the DOE labs.

ALUMNI PROFILES

FROM ALUMNI TO LEADERS

A Career at the Nuclear Intersection

Brian Moore
GE Hitachi Nuclear Energy

BRIAN MOORE's father had some tough questions for him when a Soviet nuclear reactor exploded in April 1986.

Moore was just beginning his nuclear engineering studies when the Chernobyl accident occurred, spreading radioactivity over Western Europe. The accident hobbled the entire nuclear energy industry, even though — as Moore told his father — a poor design and lax safety standards were to blame.

"I did have some heartburn from, 'Well, why are you still going into this stagnant industry?'" Moore says, but he liked the field's combination of nuclear physics, reactor engineering, applied mathematics and computational science. "It's this sort of in-between world where they all interact."

Moore, a Department of Energy Computational Science Graduate Fellowship recipient from 1992 to 1995 — part of just the second class in the program's 20-year history — has inhabited that world since earning his doctoral degree from North Carolina State University in 1996. He joined the nuclear energy arm of the General Electric Co. and now manages the Methods and Software Development Center of Excellence. He's also part of GE Hitachi Nuclear Energy, an alliance between the iconic American and Japanese companies to develop and market nuclear technology, services and fuels.

"I still feel like I'm sitting on this intersection between all these cool things," Moore says from his office in Wilmington, N.C. "I get to play in all of it. If we're doing computational fluid dynamics simulation of part of the reactor, I get to see that. If we're doing the heterogeneous full transport calculations for part of the fuel bundle, I get to play in that. If I'm getting the whole system aspect or even what happens when someone wants to do a new application, I get to play in that, too."

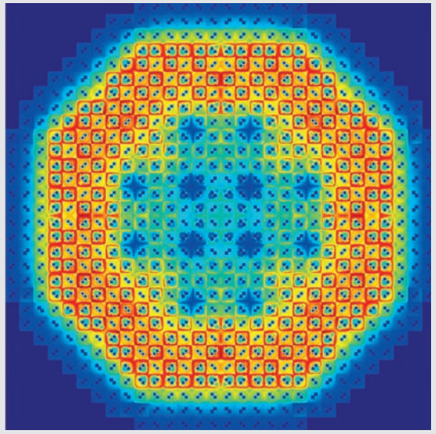
Moore and his team create predictive reactor core models, combining the physics of fission, fluid dynamics and other processes with decades of reactor operation data. The resulting calculation is fairly straightforward, Moore says. "The only problem is we can't solve it explicitly; it's too complicated and it's too big, so we end up making any number of different kinds of approximations."

To help compensate, Moore and his colleagues may couple detailed models into broad simulations. For instance, they may tie two-dimensional "slices" of fuel assemblies into a three-dimensional setting to calculate a reactor's full power distribution. The data is "in a system where we can both use it to prognosticate what the next two years might be or, in what we're required to do in licensing, what the next 5 seconds" might hold.

"After we've created these nice big physics tools [we] walk them through regulatory licensing approval," Moore says. The U.S. Nuclear Regulatory Commission (NRC) — and similar bodies in countries where GE and GE Hitachi build and service reactors — not only review reactor designs, but also mathematical tools used to estimate their capacities and limits. Regulators aren't "just concerned with, 'Is it doing the right thing?' They also want to know how you're going to use it" and whether the application is conservative enough to account for biases and uncertainties.

This cutaway drawing of the GE Hitachi Economic Simplified Boiling Water Reactor pressure vessel shows the core and other features. Brian Moore and his team at the Methods and Software Development Center of Excellence helped analyze new reactor core monitoring instruments and core and fuel properties for the design.

Image Copyright GE Hitachi Nuclear Energy.



Predicted linear heat generation rate (kW/ft) distribution across a boiling water reactor radial plane at an elevation of 21 inches from the base of active fuel early in the operating cycle. The predictive capability is verified via non-destructive fission product signature measurements. Examined for every pin at each point in the cycle and compared to the fuel design limit, the bundle and/or core design can be optimized to maximize performance while meeting all safety limits.

Image Copyright GE Hitachi Nuclear Energy.

The last nuclear plant built in the United States went on line in 1996 — the same year Moore earned his doctorate. But GE still builds in other countries and, just as importantly, helps modify existing plants for greater efficiency and capacity. Moore and his colleagues calculate the consequences of putting more fuel rods in an assembly and worked on MELLLA (Maximum Extended Load Line Limit Analysis) Plus, GE Hitachi's technology to boost output on boiling water reactors.

Moore also helped analyze new reactor core monitoring instruments and core and fuel properties in the Economic Simplified Boiling Water Reactor, which, in addition to the PRISM Advanced Recycling Center, is a leading-edge design for GE Hitachi.

And since 2000, Moore has been part of Global Nuclear Fuel, a venture linking GE, Hitachi and Toshiba. "I have the opportunity to look for areas of synergy where we can help each other out … and try to avoid duplication of effort so we can maximize the brilliant people we have."

Moore's elevation to management has given him another area to play in: spreading the word about how computational science can boost GE Hitachi's overall business. "Taking on the leadership positions has been very good for me to stretch beyond my comfort zone, and that's what I really like."

DOE CSGF graduates move to the front in their fields

Since 1991, the Department of Energy Computational Science Graduate Fellowship has seeded government laboratories, industry and academia with scientists trained to apply high-performance computing to challenging research problems. Alumni have made outstanding contributions, including improved fusion plasma models, insights into evolution of drug-resistant diseases and more efficient and economical nuclear power plant designs. More importantly, they've helped develop computer simulation and computational science into a research tool that equals theory and experiment. As these profiles show, alumni are the DOE CSGF's best promoters.

Dan Martin
Lawrence Berkeley National Laboratory

"Cool Problems" Draw Alumnus to Laboratory

It may help to think of DAN MARTIN as a carpenter whose main tool is a trusty multipurpose saw.

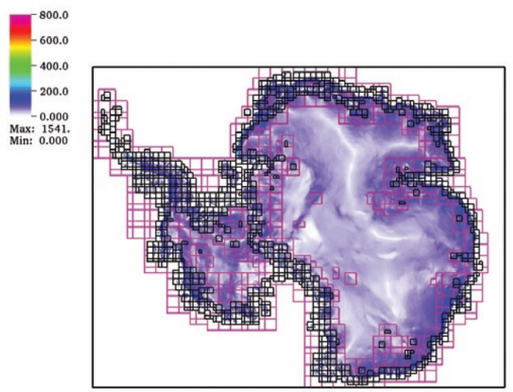
Martin, a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient from 1993 to 1996, works with scientists in a variety of fields to build computer models. He's helped fashion algorithmic "lumber" into simulations portraying devices and phenomena ranging from fusion plasmas' rapid reactions to ice sheets' glacial movements.

"It's fun to work on really cool problems," says the researcher in the Applied Numerical Algorithms Group (ANAG) at Lawrence Berkeley National Laboratory (LBNL). "That's one of the advantages of being a computational scientist. I've been all over the place. I've gotten to learn a lot about a lot of really cool and interesting areas."

The versatile tool Martin and his colleagues often use is adaptive mesh refinement (AMR), a computational technique that focuses a computer's power where it's needed most. AMR automatically casts fine, high-resolution grids or meshes of data points in areas of interest in a simulated domain — like the point where two fluids interact — and coarser meshes elsewhere. Computers calculate changes in physical properties at each data point to provide a complete picture. "You can think of AMR as giving you essentially fine-grid accuracy for essentially coarse-grid (computational) cost," Martin says.

That's just what one of Martin's latest projects needs. He and his colleagues are part of ISICLES, the Ice Sheet Initiative for CLimate ExtremeS, a DOE program to develop better models of land-based ice sheets. "Ice sheets have an enormous range of dynamic scales. You need incredibly fine resolution to get some features right," like the grounding line, the point at which an ice sheet slides off land and onto the ocean. "But there also are large regions where nothing's going on. You really can't computationally afford to resolve everything at the fine scale."

The LBNL project, called Berkeley-ISICLES or BISICLES, applies AMR to the Glimmer Community Ice Sheet Model, often a component of larger climate simulations. The team also uses other algorithmic adjustments, including approximating the vertical structure or distribution of the ice-sheet velocity and coupling it to equations for the sheet's horizontal movement and thickness evolution. That "lets us get away with a two-dimensional vertically integrated solver that's also a big win" in saving computational power.



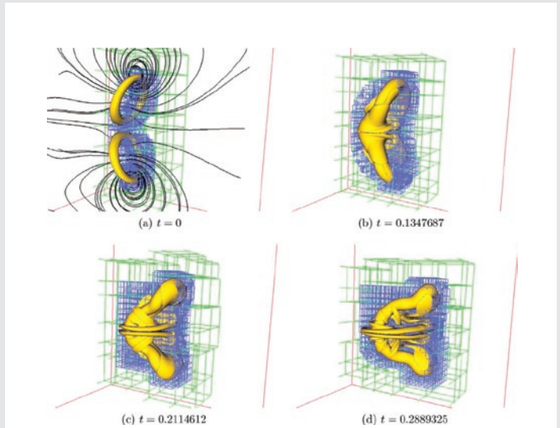
This visualization of a simulation of Antarctic ice sheet movement shows the magnitude of the ice sheet's velocity in meters per year, with blue-white the lowest velocity magnitude and blue-green higher magnitude. The visualization also shows the adaptive computational grid used to calculate the velocity magnitude. Small, black boxes have a resolution of 2.5 kilometers and purple boxes are at 5 kilometers. The base resolution for the simulation is 10 kilometers.

Martin spends a lot of time extending AMR and other algorithmic techniques to new and bigger problems. Application scientists can't "just take a problem and drop it into AMR. Everything has its own refinements and its own algorithmic complexity. Doing it correctly for any given problem often requires work and research." The Applied Numerical Algorithms Group also focuses on improving AMR to higher orders of accuracy and on finding better ways to solve the partial differential equations at the heart of computer models.

Martin also is on the development team for Chombo, an ANAG-developed software package for adaptively refined rectangular grids, and frequently answers questions from researchers who use it. "There's an impressive number of really capable people who are using our software to attack problems we don't have time or resources to look at, but are still good candidates for AMR."

One of AMR's creators, ANAG leader Phillip Colella, was his doctoral advisor at the University of California, Berkeley, but Martin says his 1994 practicum under combustion modeler and AMR pioneer John Bell was what set him on course for a laboratory career. "I really enjoyed working with the people," Martin adds. A lab career "seemed like a way to be able to do lots of fun, exciting research without having to go through the tenure process." He's also found a national laboratory is "one of the places where teamwork … just works so much better."

As LBNL's DOE CSGF practicum coordinator, Martin pairs students with researchers in complementary disciplines. "I meet people all across the lab and they think I'm great because I bring them all these fantastic people," he adds. "It's definitely improved my knowledge of what's going on at the lab in a way that's been fun."



This is a demonstration of an algorithm that uses computational meshes localized in both space and time to compute incompressible viscous flows. It shows two vortex rings angled toward each other at initial time and after 60, 90 and 120 time steps. Black lines depict streamlines. Green boxes are a level 1 mesh, with a resolution four times finer than the background mesh. Blue boxes are a level 2 mesh, with a resolution four times finer than level 1. For clarity, grid boxes are shown only in the rear half of the computational domain.

Mala Radhakrishnan
Wellesley College

Alumna Busts Resistance — in the Classroom and Lab

MALA RADHAKRISHNAN is out to override resistance. As an assistant professor of chemistry at Wellesley College, much of her research aims to outmaneuver mutations in viruses like HIV that make some drugs nearly useless.

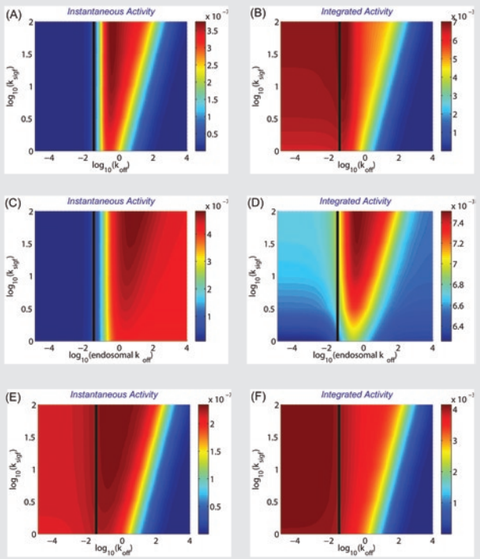
Radhakrishnan, a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient from 2004 to 2007, builds computational models for drug design. Sometimes those models design and analyze "promiscuous" molecules — ones capable of targeting multiple viral variants. Radhakrishnan also uses optimization methods to help find effective molecular combinations to block many variants with minimal side effects. And in current research she's searching for common factors in HIV drug resistance.

Just as importantly, Radhakrishnan is sharing her expertise and setting a standard for Wellesley students. She found she was at home in the classroom while participating in the Teach for America program after earning her undergraduate degree.

"During grad school I actually missed teaching. That's another reason I knew academia would probably be a better fit for me," Radhakrishnan says. "The teaching, the mentorship is the best part," whether it's a chemistry class or writing computer code. "It's really fun for me to see a student who has never written a piece of code before get excited when something works."

That's an especially vital message at Wellesley, Radhakrishnan says. Teaching at a women's college is important because "there still aren't enough female computational scientists out there" — something she and her students are reminded of every time they attend a conference or take a job.

At Wellesley, Radhakrishnan carries out most of her projects on a computing cluster with 80 processing cores, but she's contemplating bigger computers soon, when she takes a year off from teaching to focus solely on research.



Results of simulations to determine instantaneous and integrated cytokine activity at 15,000 minutes as a function of surface/endosomal dissociation rate constant (k_{off}) and activation rate constant with a liganded receptor (k_{sigf}). Figures (A) and (B) are for endosomal k_{off} and k_{sigf} for parameters similar to those for the cytokine Granulocyte-colony stimulating factor (GCSF). Figures (C) and (D) show activity and integrated activity as a function of endosomal k_{off} and k_{sigf} for the same parameters, with surface k_{off} held fixed to reflect mutant GCSF with poorer binding only in the endosome. The alteration further maximizes instantaneous and integrated activity. Figures (E) and (F) show plots for instantaneous and integrated activity for k_{off} and k_{sigf} under parameters similar to those for the cytokine Erythropoietin (Epo). The plots show that tighter binders were consistently preferred in the Epo system. In all cases the black line indicates the experimentally measured k_{off} at cell surface pH.

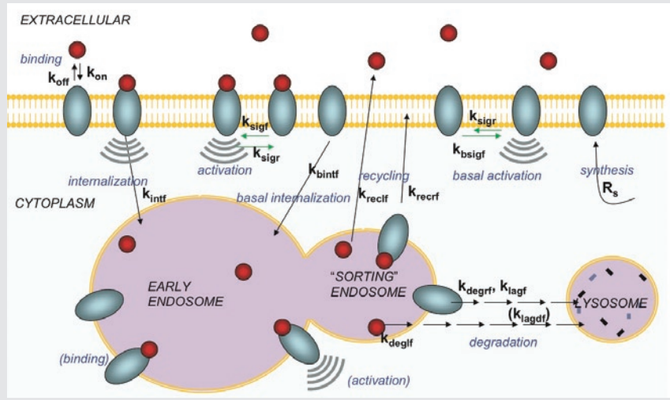
She's already compiled a strong record of achievement. In a paper published last year in the journal *Biotechnology Progress*[1], Radhakrishnan and Bruce Tidor, her doctoral advisor at the Massachusetts Institute of Technology (MIT), computationally varied the binding behavior of cytokines, proteins that attach to cells to regulate them. Erythropoietin (Epo), for instance, binds to surface receptors to regulate red blood cell maturation.

Radhakrishnan and Tidor modeled how changing the time cytokines bind to their receptors could affect their longer-term potency. The longer a cytokine remains bound, the more likely it is to be internalized and degraded, making it unavailable to bind at another receptor. Their model indicated that a weakly binding cytokine works better when less of it is available or when cells quickly internalize and degrade it, for example. In those cases the cytokine releases from the receptor and is recycled for binding at another site. Strongly binding cytokines are better in other situations — when they activate slowly or when the cell has fewer receptors.

"A lot of researchers, when they design drugs, they want things to bind as tightly as possible," Radhakrishnan says. "This shows an example where that can be a detriment. You lose the long-term potency."

It took a large-scale cellular model to test that idea. In other research Radhakrishnan used molecular-scale models to design two mutant Epo receptors. The receptors selectively bound to one of two different parts of the Epo molecule, letting Radhakrishnan and her MIT colleagues explore how selective binding affects cell response.

Radhakrishnan takes an equally small-scale approach in a collaboration with fellow DOE CSGF alumnus Jaydeep Bardhan. Bardhan, an assistant professor at Rush University Medical Center in Chicago, has developed a way to efficiently calculate electrostatics — electrical charges and fields — that influence biomolecules. "I'm working with him to try to apply it to biological systems and see in what cases it works well and when it doesn't," Radhakrishnan adds. It could lead to simulations that better capture the fine detail of biochemical interactions.



Mala Radhakrishnan and Bruce Tidor built a computational model of cytokine behavior illustrated here. Cytokines are small proteins that bind to specific cell surface receptors. Cytokines may bind to receptors to activate a signal in the cell, then release to bind at another site. Others are brought into the cell where they may remain activated before they are recycled back to the cell surface or degraded in the lysosome.

At the other end of the scale, Radhakrishnan is working with Stanford University medical researcher Robert Shafer to analyze a database of HIV drug-resistance data. "I'm looking for patterns and trying to understand what major drug-resistant genotypes and phenotypes are out there," she says. "Is there a set of representative ways a person could be resistant to HIV drugs?" By identifying key drug-resistance factors, researchers could design "promiscuous" new drugs or drug cocktails with multiple infection targets.

Radhakrishnan will focus on new challenges during her year of research. Meanwhile, she's also tending to her infant son, Samay, and recently published a collection of "chemistry poetry" entitled *Atomic Romances, Molecular Dances.*

[1] Radhakrishnan ML, Tidor B. Cellular-level models as tools for cytokine design. *Biotechnol Prog.* 2010;26:919-937.

WINNING ESSAYS

ENCOURAGING COMMUNICATION THROUGH AN ANNUAL WRITING CONTEST

WINNER

by Kenley Pelzer

CAN PEELING AN ONION CURE CANCER?

AWARDING COMMUNICATION

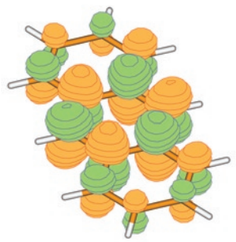
The DOE CSGF launched an annual essay contest in 2005 to give current and former fellows an opportunity to write about their work with a broader, non-technical audience in mind. The competition encourages better communication of computational science and engineering and its value to society to non-expert audiences.

In addition to recognition and a cash prize, the winners receive the opportunity to work with a professional science writer to critique and copy-edit their essays. The latest winning essays are published here.

For more information on the essay contest, visit www.krellinst.org/csgf.

"WITH NO OFFENSE to the quantum theorist in the room," the professor said, casting me a quick look and smiling gently, "you should never, ever deal with quantum effects unless you have to." As an eager young graduate student in theoretical quantum chemistry, I was enthralled by the wonderful and bizarre laws Einstein and other great scientists had discovered. Yet I knew the professor had a point: If you unnecessarily involve these strange principles in your approach to a scientific problem, it will be harder — or perhaps impossible — to solve it.

In the world of quantum mechanics, objects behave in very peculiar ways. An object can pass through walls. It can be in two places at the same time. No matter how hard you try, you can never be sure where it is or where it is going. Fortunately for scientists, these quantum effects are only important for the smallest particles and can be ignored in many situations.



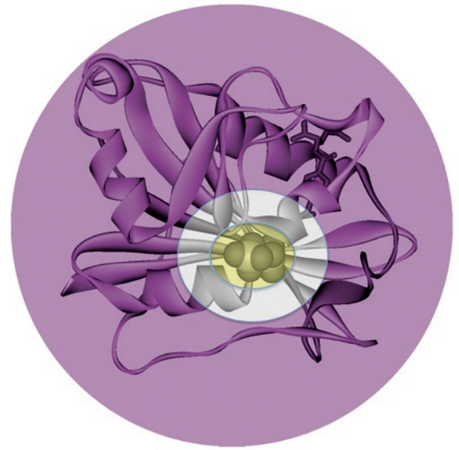
This image shows a molecular orbital calculated using a quantum mechanics program. By calculating the shapes and orientations of the molecular orbitals, which may contain electrons, scientists obtain detailed information on the distribution of the electrons in space.

However, it is absolutely crucial to consider quantum theory in some cases, because its messy, complicated rules can help us understand diseases — and how to cure them.

The human body contains a multitude of protein molecules that play a central role in whether we stay healthy or get sick. Each protein contains thousands of electrons — tiny, negatively charged particles that are attracted to positive charges. These attractions influence whether a protein "sticks" to another molecule.

This biological stickiness is especially important in treating cancer. In some types of cancer cells, there are protein molecules with a region called an "active site." When certain molecules attach to the active site, they trigger a cascade of events that leads to disease. But if a drug can target a particular protein and stick to its active site, it can block other molecules from binding and prevent this dangerous spiral. If a drug can't stick to the protein — if it falls off and circulates in the bloodstream — it may just float around doing nothing or, worse yet, cause toxic side effects.

To predict which drugs will attach firmly to an active site, scientists must understand how protein molecules and their electrons behave. But because electrons are so small, they obey all of the complicated laws of quantum mechanics.



Pictured here is dihydrofolate reductase, a protein whose function is crucial for cell proliferation. Drugs that bind to the active site of this protein and inhibit its activity are used to stop the rapid proliferation of cancer cells. The yellow shaded region surrounds the active site.

So how can anyone possibly study a protein with thousands of these slippery, mysterious little particles?

Since electrons are too small to see through a microscope, chemists predict their behavior with sophisticated computer simulations. Not only do these simulations have the power to study electrons, they also have economic advantages: Once the software has been developed, it costs virtually nothing to use it to study large numbers of potential drugs. Given the massive costs involved in pharmaceutical research, this advantage has important implications in the search for effective medicines.

The bad news is that — thanks to the influence of quantum properties — these simulations may take weeks to generate information about just a few electrons. Since a protein has thousands, accurately predicting the distribution of electrons could take decades. Not very helpful when cancer patients are hoping for a new drug *now*.

This is where the idea of peeling an onion comes to the rescue. With the aptly named ONIOM method ("Our own N-layered Integrated molecular Orbital molecular Mechanics") the protein molecule is divided into a chosen number (N) of layers. The program treats each with a different simulation technique, carefully selected based on what information is needed. When highly accurate information on the electronic structure is needed, the program uses a "molecular orbital" method that rigorously incorporates quantum theory. The details of quantum theory are so important for these molecular orbital calculations that they are usually referred to as "quantum mechanics" calculations.

When a lower level of accuracy is acceptable for a particular layer, the program may use a less advanced (and less time-consuming) quantum mechanics method. In cases where even more approximate information is sufficient, the computer performs a "molecular mechanics" calculation. Because molecular mechanics methods are less precise and incorporate less quantum mechanical theory, they're fast — really fast. So by applying molecular mechanics and working with information that's a little less accurate, the simulations gain a lot of speed.

To understand how the ONIOM approach can help us answer important questions, consider the example of a drug that needs to bind to a particular protein. At the protein's active site — the onion's center — the computer uses an advanced quantum mechanics method to calculate the behavior of electrons and predict whether a drug will "stick."

Then the computer must simulate the next layer of the onion — or rather, the next layer of the protein — which wraps around the active site but isn't part of the active site. Since this layer doesn't actually stick to the drug of interest, we don't need to worry quite as much about its electrons. On the other hand, we can't totally ignore this layer, because changes in its shape or electron distribution might affect the active site's behavior. So scientists compromise and use a less precise method: either a quantum mechanics method that is a little less accurate (and hence faster), or a molecular mechanics method.

The farther we are from the active site, the less we need detailed information about electrons and their quantum mechanical behavior. So we use a less precise simulation technique with each successive layer. By using faster techniques to treat the outer layers of the "onion," it's possible to predict how a large protein will interact with a particular drug. And fortunately for patients waiting for the next new medicine, the answers can be obtained in days or weeks — not decades.

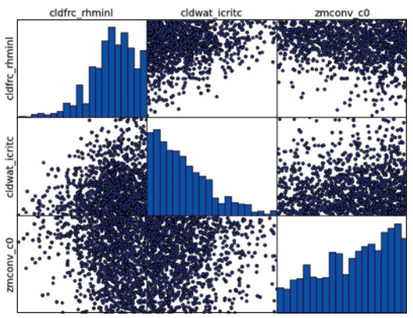
By peeling apart a protein as though it were an onion, scientists follow my professor's advice to never, ever deal with quantum effects unless you have to. The beauty of this approach is that for many physiological proteins, neither quantum mechanics nor molecular mechanics alone could effectively answer our questions. Fortunately, collaboration between scientists who specialize in each method has led to ingenious hybrid programs that can contribute great insights to drug design. And then with the press of a key, a computer can guide us in the urgent quest to develop life-saving medicines.

HONORABLE MENTION

ON THE QUANTIFICATION OF "MAYBE": A NICHE FOR COMPUTATION

by Hayes Stripling

Each column of the figure illustrates a calibrated or posterior distribution of a single uncertain input to a massive climate model. The bar charts (histograms) represent the single-variable distribution and the scatter plots illustrate how the calibration of one variable correlates to the other two variables. For example, these results suggest larger values of cldfrc_rhminl and smaller values of cldwat_icritc will improve the accuracy and reduce uncertainty in future model runs.



CONSIDER PERHAPS THE MOST pressing question facing the global community in this and coming decades: "Is human activity adversely affecting the environment and global climate?" A brief skimming of newspaper headlines, scholarly journals and political debates reveals that credible responses to this "yes/no" question all have a flavor of "probably," "maybe" or "probably not." In fact, most scientifically based stances concede we cannot provide a definitive "yes/no" answer without many more years' worth of data, investigation and discovery. So the correct answer today is just "maybe," with some evidence and proponents on either side.

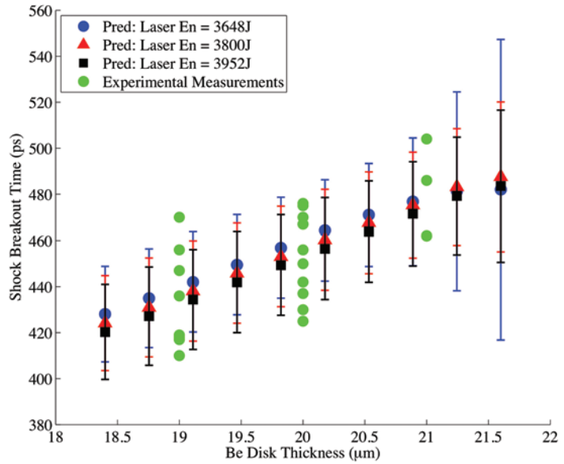
In response to scientific and political pressure for a more definitive answer, researchers have focused on this reformulation of the question: "To what extent does human activity affect the environment and global climate, and how do we manage the risks of this activity as the scientific investigation continues?" This is not posed as a "yes/no" question; instead, it calls for a quantification of "maybe" — an estimation of uncertainty in our response. Answering the question also requires a multidisciplinary effort — involving experts in science, engineering and policy development — that will evolve as we gain understanding.

These kinds of questions have led to an exploding demand for knowledge. In reaction, researchers are expanding the scientific method, which is founded on the long-lived pillars of theory and experiment, to explore new domains and strategies to support decisions and conclusions. These include computation, an invaluable tool many now accept as the third pillar of science. Using computational power to simulate a system or experiment is relatively inexpensive and has increasing potential to provide accurate, thorough results. Most importantly, computation also has surfaced as the most valuable tool for exploring uncertainty in "yes/no" questions.

The specific branch of computation that addresses this issue is uncertainty quantification (UQ). UQ — or the quantification of maybe — aims to comprehend how uncertainty in nature affects a particular quantity of interest (QOI). It then uses this understanding to make predictions or informed decisions about the quantity. Achieving this goal, however, is not so simple, for the QOIs we seek are complex results of multidisciplinary systems that are confounded by uncertain inputs and less-than-perfectly-understood physics.

To illustrate the utility of computation in uncertain systems, let's consider a simple example: determining the forces a passenger experiences in a car crash. Imagine we can identify the five most important factors (such as speed or seat-belt use) contributing to our QOI but that we can't know exactly what the settings or statuses of these inputs will be (that is, our inputs are uncertain). If we restrict each input to one of two settings (for example, speed is either fast or slow) and wish to test each possible combination of inputs, we would require the design, construction, crashing and analysis of 2^5 (32) test cars. This may be an acceptable number of experiments, depending on economic, administrative and/or political constraints. But five inputs probably are too few. A more realistic approach may consider 15 inputs — that's

The error bars represent predictions (with uncertainty) of the time required for laser energy to ablate a beryllium disk. We use existing experimental data to "tune" our uncertain parameters and reduce the magnitude of the predictive uncertainty. The analysis shows that between experimental results, the error bars are comparable to the experimental variability. Predictions at extrapolated (larger) disk thicknesses, however, are less informed by the experimental results and have larger uncertainty.



2^{15}, or 32,768 experiments — certainly a number too expensive and time-consuming to consider.

Computation has proven extremely valuable in such cases, in which experimentation is economically or politically infeasible. What if we can afford only five crash tests? We may approach the problem computationally instead. The computer model would solve equations that govern (or simulate) the physics that take place during a crash. We could design the model to accept any number of adjustable inputs that contribute to the final QOI (in this case, the forces a passenger experiences). Inputs could span a range instead of adhering to a binary choice, like fast or slow speed. It would be common, given sufficient computer resources, to run hundreds or thousands of "computer experiments" corresponding to hundreds or thousands of input combinations. The final result is a distribution of our QOI, allowing us to make an informed statement of the form, "We are 99 percent certain that the passenger G-force will be below the injury threshold in 99.9 percent of vehicle collisions." Such a statement is much more useful to a policy-making board or consumer than results from only a handful of experiments.

Cutting-edge simulations running on some of the largest computer architectures in the world use this kind of approach to address society's toughest challenges. But in some cases, the problems are becoming too large and complex. For example, models designed to describe the long-term global climate predict thousands of quantities of interest from thousands of uncertain inputs. To help handle data of this magnitude we employ sensitivity analysis, a sub-discipline of uncertainty quantification. By sampling results from previous computer experiments we can determine which outputs are most sensitive to which inputs. For example, if we find that the computed prediction of global surface temperature isn't sensitive to lunar cycles but is highly sensitive to cloud coverage, we can adapt our sampling strategies to explore cloud coverage more thoroughly and hold off on varying the lunar effects. This will give us a more precise understanding of global surface temperature behavior and use fewer evaluations of the (potentially time-consuming) computer model. It's also something we could never determine using physical experiments alone.

Of course, it's impossible for computation to ever make experimentation a moot practice. We must compare experimental measurements with computational results to ensure our models are valid. Further, experimentation's maturity as a technique and the ability to witness its physical results with your own eyes makes it more credible to humans than computational number crunching. For example, let's return to our car crash case: Would you be more inclined to believe a vehicle's safety report based on five physical experiments using real crash-test dummies or 1,000 simulated smash-ups in which you can't see, hear or feel the impact? Would you be more inclined to believe the computer if it exactly predicted the results of the five physical crashes we could afford? We can never abandon experimentation — but we can leverage validated computer models to develop and explore scientific concepts that will guide our society's policies in the face of the great challenges ahead.

The Frederick A. Howes Scholar in Computational Science award was established in 2001 to honor the late Frederick Anthony Howes, who was a champion for computational science education.

HOWES AWARD

HONORS LEADERSHIP AS WELL AS SCHOLARSHIP

2011 WINNER ALEJANDRO RODRIGUEZ

Alejandro Rodriguez has been selected as the 2011 Howes Scholar in Computational Science. Dr. Rodriguez was a fellow from 2006 to 2010. He received his Ph.D. from the Massachusetts Institute of Technology and currently holds joint postdoctoral positions at the Harvard School of Engineering and Applied Sciences and at the MIT Department of Mathematics.

A Cuban émigré who has helped scientists better understand a strange physical force is the 2011 Frederick A. Howes Scholar in Computational Science.

The award recognizes outstanding recent doctoral graduates of the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) program. Winners are chosen not just for their technical achievements, but also for outstanding leadership, integrity and character — qualities that brought Howes wide admiration.

As manager of DOE's Applied Mathematical Sciences Program, Howes was a staunch defender of the fellowship and its goals. He died unexpectedly on Dec. 4, 1999, at age 51.

Alejandro Rodriguez, a fellow from 2006 to 2010, is the 15th Howes Scholar. Rodriguez graduated from the Massachusetts Institute of Technology (MIT) in June 2010. He's now a postdoctoral researcher with a joint appointment in the Harvard School of Engineering and Applied Sciences and the MIT Department of Mathematics.

"To be honored for my work and, most importantly, for my devotion to science is not only a tremendous honor but also an invaluable source of encouragement," Rodriguez says.

2010 Howes Scholar Julianne Chung also felt invigorated. She was chosen, in part, for her work supporting budding scholars through groups such as the Association for Women in Mathematics and the Society for Industrial and Applied Mathematics. She's continued that involvement, but "with the award I feel more empowered, in that it's not just my experience I'm sharing with students. It's also Dr. Howes' vision for computational, interdisciplinary research, as well as the greater computational science community, that I represent."

Since earning her doctoral degree from Emory University in 2009, Chung completed a National Science Foundation Mathematical Sciences Postdoctoral Research Fellowship at the University of Maryland at College Park. This fall she starts a tenure-track position in the Mathematics Department at the University of Texas at Arlington, where she'll continue her work on inverse problems and image processing.

"To be honored for my work and, most importantly, for my devotion to science is not only a tremendous honor but also an invaluable source of encouragement."

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The Howes award occasionally attracted attention as Chung interviewed for positions. A faculty member at one major research university told her he'd known Howes personally. "In some sense, it was an immediate acknowledgement of the value of my research, as well as the importance of my work," she adds. "It definitely has an effect on the connection I have with the community."

DOE CSGF recipients who have completed or plan to complete requirements for their doctoral degree in a calendar year, both with fellowship support or after receiving support for the maximum number of years, are eligible for that year's Howes award. They're nominated by department chairs, advisors and fellowship coordinators at their universities. A review

Above left: 2010 winner Julianne Chung receives her award from Dr. David Brown, chair of the Howes selection committee and longtime friend of the fellowship.
Above right: David Potere, the 2009 Howes Scholar, presents his research at the DOE CSGF Annual Conference in Washington.

ABOUT FRED HOWES

In the 10 years since it was first conferred, the Frederick A. Howes Scholar in Computational Science award has become emblematic of research excellence and outstanding leadership. It's a fitting tribute to Howes, who was known for his scholarship, intelligence and humor.

Howes earned his bachelor's and doctoral degrees in mathematics at the University of Southern California, an obituary on the Society of Industrial and Applied Mathematics website reports. He held teaching posts at the universities of Wisconsin and Minnesota before joining the faculty of the University of California, Davis, in 1979. Ten years later Howes served a two-year rotation with the National Science Foundation's Division of Mathematical Sciences. He joined DOE in 1991.

In 2000, colleagues formed an informal committee to honor Howes. They chose the DOE CSGF as the vehicle and gathered donations, including a generous contribution from Howes' family, to endow an award in his name.

PAST HOWES SCHOLARS

2010	Julianne Chung
2009	David Potere
2008	Mala Radhakrishnan
2007	Jaydeep Bardhan and Kristen Grauman
2006	Matthew Wolinsky and Kevin Chu
2005	Ryan Elliott and Judith Hill
2004	Collin Wick
2003	Oliver Fringer and Jon Wilkening
2001	Mayya Tokman and Jeffrey Hittinger
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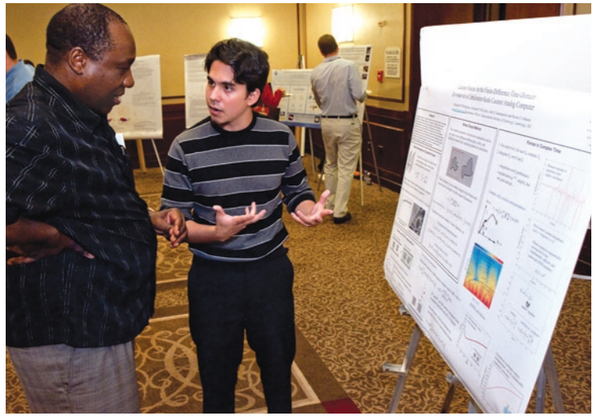

Alejandro Rodriguez, the 2011 Howes Scholar in Computational Science, explains his research and award-winning poster at the 2009 annual conference.

committee chooses one or two scholars each year to receive an honorarium and engraved crystal memento at the DOE CSGF Annual Conference in Washington, D.C., where the recipients also deliver lectures describing their research.

David Potere, the 2009 Howes Scholar, said the talk was one of the honor's most significant elements. At Princeton University he focused on applying computer power to analyze the huge quantity of data remote sensing satellites generate, using it for things like predicting epidemics. His Howes lecture focused on what the satellites see.

"I was hoping to just leave the room with a sense of how beautiful the remote sensing satellite imagery is and how much things are changing," Potere says. "We're really at a tipping point now." After graduation he joined the Boston Consulting Group, where he's helped found a "geoanalytics team." It plans to apply geospatial technologies to problems such as store location, demographics and distribution optimization.

Potere says the Howes award surprised him because "I hadn't really thought of myself that way." Yet, like Chung, he found "it was a nice piece of confirmation that there was a leadership impact and a leadership role" to his research.

For Rodriguez, the honor has special meaning "after spending the past five years in the company of extremely talented and passionate CSGF fellows."

Rodriguez, the selection committee wrote in its citation, "embodies the qualities that Fred Howes promoted in all young scientists." He is "not just an exemplary computational physicist," but also "a dedicated spokesman for physics and a mentor for younger scientists." Rodriguez taught physics in the MIT summer MITES program for under-represented high school students. He also has represented both the MIT physics department and DOE CSGF at national conferences and is profiled in the Physics Society "People in Physics" video series.

"I love to share my work and passion for science with others," Rodriguez says. "The less the audience knows or cares about science, the more I enjoy convincing them of its importance and beauty." The award recognizes the significance of mentorship and scholarship, he adds, and he plans to use it "as fuel to continue to inspire others."

Rodriguez's research has led the way in understanding the Casimir forces. These strange attractions arise from quantum-scale fluctuations in the electromagnetic field and are affecting microelectromechanical systems now in development. Rodriguez's work has led to methods capable of calculating these forces between arbitrarily shaped objects. Previous techniques could only predict them between simply shaped objects. Rodriguez is first author on numerous papers describing the research, including ones published in the *Proceedings of the National Academy of Sciences* and *Physical Review Letters*.

Rodriguez was 13 when he and his family fled Cuba after his stepfather, a physics professor, was fired for refusing to identify the writers of a letter opposing the communist government. They settled in the Miami area and became U.S. citizens.

The award, Rodriguez says, recognizes the role his entire family, including those still in his native land, had in his success. Naturally, they're overjoyed: "My father in Cuba almost went as far as publishing the news in the national Cuban newspaper."

2011 fellows directory
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Cornell University
Computational Materials Physics
Fellowship Years: 1991-1995
Current Status: Drupal Developer, Cronen-Townsend Consulting

Robert Cruise
Indiana University
Computational Physics
Fellowship Years: 1997-2001
Current Status: Department of Defense

Aron Cummings
Arizona State University
Nanoscale Electronics
Fellowship Years: 2003-2007
Current Status: Postdoctoral Researcher, Sandia National Laboratories – California

Joseph Czyzyk
Northwestern University
Industrial Engineering and Management
Fellowship Years: 1991-1994
Current Status: Business Intelligence Analyst, Central Michigan University Research Corporation

Tal Danino
University of California, San Diego
Dynamics of Systems Biology
Fellowship Years: 2006-2010
Current Status: Postdoctoral Researcher, Boston University/Massachusetts Institute of Technology

William Daughton
Massachusetts Institute of Technology
Plasma Physics
Fellowship Years: 1992-1996
Current Status: Staff Scientist, Los Alamos National Laboratory

Gregory Davidson
University of Michigan
Nuclear Engineering and Computational Science
Fellowship Years: 2002-2006
Current Status: Oak Ridge National Laboratory

Jimena Davis
North Carolina State University
Uncertainty Quantification, Physiologically Based Pharmacokinetic Modeling, Risk Assessment
Fellowship Years: 2004-2008
Current Status: Postdoctoral Fellow, U.S. Environmental Protection Agency

Jack Deslippe
University of California, Berkeley
Computational Condensed Matter Theory
Fellowship Years: 2006-2010
Current Status: Graduate Student

Mark DiBattista
Columbia University
Computational Fluid Dynamics
Fellowship Years: 1992-1994

John Dolbow
Northwestern University
Computational Methods for Evolving Discontinuities and Interfaces
Fellowship Years: 1997-1999
Current Status: Yoh Family Professor, Duke University

Laura Dominick
Florida Atlantic University
Computational Electromagnetics/ Electromagnetic Performance of Materials
Fellowship Years: 1993-1997
Current Status: Large Military Engines Division, Pratt & Whitney

Michael Driscoll
Boston University
Bioinformatics and Systems Biology
Fellowship Years: 2002-2006
Current Status: Dataspora Inc.

Jeffrey Drocco
Princeton University
Biophysics and Computation
Fellowship Years: 2004-2008
Current Status: Postdoctoral Researcher, Los Alamos National Laboratory

Brian Dumont
University of Michigan
Aerospace Engineering
Fellowship Year: 1994
Current Status: Airflow Sciences Corporation

Amanda Duncan
University of Illinois at Urbana-Champaign
Electrical Engineering
Fellowship Years: 1991-1995
Current Status: Senior Staff Engineer, Intel Corporation

Mary Dunlop
California Institute of Technology
Bioengineering, Synthetic Biology, Biofuels, Dynamical Systems
Fellowship Years: 2002-2006
Current Status: Assistant Professor, University of Vermont

Lewis Dursi
University of Chicago
Computational Astrophysics, Large-Scale Simulation, Hydrodynamics, Combustion, Magnetohydrodynamics
Fellowship Years: 1999-2003
Current Status: Senior Research Associate, CITA

Ryan Elliott
University of Michigan
Shape Memory Alloys and Active Materials
Fellowship Years: 2000-2004
Current Status: Assistant Professor, Department of Aerospace Engineering and Mechanics, University of Minnesota

Thomas Epperly
University of Wisconsin
Component Technology for High-Performance Computing
Fellowship Years: 1991-1995
Current Status: Lawrence Livermore National Laboratory

Susanne Essig
Massachusetts Institute of Technology
Aeronautics and Astronautics, Computational Turbulence
Fellowship Years: 1997-2002

Annette Evangelisti
University of New Mexico
Computational Molecular Biology
Fellowship Years: 2001-2005
Current Status: Postdoctoral Researcher, University of New Mexico

John Evans
University of Texas
Computational and Applied Mathematics
Fellowship Years: 2006-2010
Current Status: Graduate Student

Matt Fago
California Institute of Technology
Computational Structural Mechanics
Fellowship Years: 2000-2003
Current Status: Research Scientist

Michael Falk
University of California, Santa Barbara
Stress-Driven Materials Processes Including Fracture, Deformation and Semiconductor Crystal Growth
Fellowship Years: 1995-1998
Current Status: Associate Professor, Materials Science and Engineering, Johns Hopkins University

Matthew Farthing
University of North Carolina
Flow and Transport Phenomena in Porous Media
Fellowship Years: 1997-2001
Current Status: Research Hydraulic Engineer, Coastal and Hydraulics Laboratory, U.S. Army Corps of Engineers Engineer Research and Development Center

Michael Feldmann
California Institute of Technology
Computational Finance
Fellowship Years: 1999-2002
Current Status: Executive Vice President, Quantitative Research, Walleye Trading Software LLC

Krzysztof Fidkowski
Massachusetts Institute of Technology
Computational Fluid Dynamics
Fellowship Years: 2003-2007
Current Status: Assistant Professor, Aerospace Engineering, University of Michigan

Piotr Fidkowski
Massachusetts Institute of Technology
Structural/Computational Engineering
Fellowship Years: 2009-2011
Current Status: Software Engineer, Google Inc.

Stephen Fink
University of California, San Diego
Computer Science
Fellowship Years: 1994-1998
Current Status: IBM

Robert Fischer
Harvard University
Security, Privacy, Mobile Agents, Software Engineering
Fellowship Years: 1994-1998
Current Status: Quant

Jasmine Foo
Brown University
Applied Mathematics
Fellowship Years: 2004-2008
Current Status: Postdoctoral Fellow, Harvard University

Ashlee Ford
University of Illinois at Urbana-Champaign
Modeling of Drug Delivery, Numerical Methods for Partial Differential Equations
Fellowship Years: 2006-2010
Current Status: Graduate Student

Gregory Ford
University of Illinois at Urbana-Champaign
Chemical Engineering
Fellowship Year: 1993

Robin Friedman
Massachusetts Institute of Technology
Computational and Systems Biology
Fellowship Years: 2007-2010
Current Status: Postdoctoral Fellow, Institut Pasteur

Oliver Fringer
Stanford University
Parallel Coastal Ocean Modeling
Fellowship Years: 1997-2001
Current Status: Assistant Professor, Stanford University

Kenneth Gage
University of Pittsburgh
Molecular Imaging, Computational Fluid Dynamics Design of Artificial Organs
Fellowship Years: 1998-2002
Current Status: Radiology Resident (Research Track), Johns Hopkins Medical Institutions

Nouvelle Gebhart
University of New Mexico
Chemistry
Fellowship Years: 2001-2003
Current Status: Deceased

Sommer Gentry
Massachusetts Institute of Technology
Optimization
Fellowship Years: 2001-2005
Current Status: Assistant Professor, Mathematics, U.S. Naval Academy

Charles Gerlach
Northwestern University
Finite Elements, High Strain Rate Solid Mechanics
Fellowship Years: 1995-1999
Current Status: Southwest Research Institute

Timothy Germann
Harvard University
Physical Chemistry
Fellowship Years: 1992-1995
Current Status: Staff Member, Los Alamos National Laboratory

Christopher Gesh
Texas A&M University
Computational Transport Theory, Nuclear Reactor Analysis, Nuclear Non-Proliferation
Fellowship Years: 1993-1997
Current Status: Pacific Northwest National Laboratory

Matthew Giamporcaro
Boston University
Adaptive Algorithms, Artificial Neural Networks
Fellowship Years: 1998-2000
Current Status: Engineering Consultant, GCI Inc.

Ahna Girshick
University of California, Berkeley
Computational Models of Vision and Perception
Fellowship Years: 2001-2005
Current Status: Postdoctoral Researcher, University of California, Berkeley

Kevin Glass
University of Oregon
Computational Ecology
Fellowship Years: 1996-2000
Current Status: Scientist, Molecular Science Computing Facility, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory

Larisa Goldmints
Carnegie Mellon University
Structural and Computational Mechanics
Fellowship Years: 1997-2001
Current Status: General Electric; Rensselaer Polytechnic Institute

William Gooding
Purdue University
Chemical Engineering
Fellowship Years: 1991-1994

Kristen Grauman
Massachusetts Institute of Technology
Computer Vision, Machine Learning
Fellowship Years: 2001-2005
Current Status: Clare Boothe Luce Assistant Professor, Department of Computer Science, University of Texas at Austin

Corey Graves
North Carolina State University
Pervasive Computing/Image Processing
Fellowship Years: 1996-2000
Current Status: Business Owner, Scholars' Advocate; Assistant Professor, North Carolina A&T State University

Michael Greminger
University of Minnesota
Mechanical Engineering
Fellowship Years: 2002-2005
Current Status: Seagate Technology

Noel Gres
University of Illinois at Urbana-Champaign
Electrical Engineering
Fellowship Years: 1999-2001

Boyce Griffith
New York University
Mathematical Modeling and Computer Simulation in Cardiac and Cardiovascular Physiology
Fellowship Years: 2000-2004
Current Status: Assistant Professor of Medicine, Leon H. Charney Division of Cardiology, New York University School of Medicine

Eric Grimme
University of Illinois at Urbana-Champaign
Electrical Engineering
Fellowship Years: 1994-1997
Current Status: Intel Corporation

John Guidi
University of Maryland
Computer Science
Fellowship Years: 1994-1997
Current Status: High School Math Teacher

Brian Gunney
University of Michigan
Computational Fluid Dynamics, Multi-Physics Simulations, Adaptive Mesh Refinement, Parallel Computing
Fellowship Years: 1993-1996
Current Status: Lawrence Livermore National Laboratory

Aric Hagberg
University of Arizona
Applied Mathematics
Fellowship Years: 1992-1994
Current Status: Staff Member, Los Alamos National Laboratory

Glenn Hammond
University of Illinois at Urbana-Champaign
Multiphase Flow and Multicomponent Biogeochemical Transport, Parallel Computation
Fellowship Years: 1999-2003
Current Status: Scientist III, Pacific Northwest National Laboratory

Jeff Hammond
University of Chicago
Supercomputing, Computational Chemistry, Programming Models, Verification and Validation
Fellowship Years: 2005-2009
Current Status: Director's Postdoctoral Fellow, Argonne Leadership Computing Facility

Jeff Haney
Texas A&M University
Physical Oceanography
Fellowship Years: 1993-1996
Current Status: IT Manager, Dynacon Inc.

Heath Hanshaw
University of Michigan
High Energy Density Physics
Fellowship Years: 2001-2005
Current Status: Sandia National Laboratories – New Mexico

Rellen Hardtke
University of Wisconsin
Particle Astrophysics (Neutrinos from Gamma-Ray Bursts), Gender and Science
Fellowship Years: 1998-2002
Current Status: Associate Professor, University of Wisconsin-River Falls

Kristi Harris
University of Maryland, Baltimore County
Theoretical Solid State Physics
Fellowship Years: 2006-2010
Current Status: Analyst, Department of Defense

Owen Hehmeyer
Princeton University
Chemical Engineering
Fellowship Years: 2002-2006
Current Status: ExxonMobil Upstream Research Corporation

Eric Held
University of Wisconsin
Plasma/Fusion Theory
Fellowship Years: 1995-1999
Current Status: Associate Professor, Physics Department, Utah State University

Asegun Henry
Massachusetts Institute of Technology
Renewable Energy, Atomistic Level Heat Transfer, First Principles Electronic Structure Calculations
Fellowship Years: 2005-2009
Current Status: Fellow, Advanced Research Projects Agency – Energy, U.S. Department of Energy

Judith Hill
Carnegie Mellon University
Computational Fluid Dynamics, Partial Differential Equation-Constrained Optimization
Fellowship Years: 1999-2003
Current Status: Computational Mathematics, Oak Ridge National Laboratory

Charles Hindman
University of Colorado
Aerospace Engineering
Fellowship Years: 1999-2003
Current Status: Air Force Research Laboratory, Space Vehicles Directorate

Jeffrey Hittinger
University of Michigan
Computational Plasma Physics
Fellowship Years: 1996-2000
Current Status: Staff Member, Center for Applied Scientific Computing, Lawrence Livermore National Laboratory

Gordon Hogenson
University of Washington
Physical Chemistry
Fellowship Years: 1993-1996
Current Status: Technical Writer, Microsoft

Daniel Horner
University of California, Berkeley
Breakup Processes, Quantum Molecular Dynamics
Fellowship Years: 2000-2004
Current Status: Research Analyst, Advanced Technology and Systems Analysis Division, Center for Naval Analysis

William Humphrey
University of Illinois at Urbana-Champaign
Physics
Fellowship Years: 1992-1994
Current Status: NumeriX LLC

Jason Hunt
University of Michigan
Aerospace Engineering and Scientific Computing
Fellowship Years: 1999-2003
Current Status: General Dynamics – Advanced Information Systems

E. McKay Hyde
California Institute of Technology
Efficient, High-Order Integral Equation Methods in Computational Electromagnetics and Acoustics
Fellowship Years: 1999-2002
Current Status: Assistant Professor, Computational and Applied Mathematics, Rice University

Eugene Ingerman
University of California, Berkeley
Applied Mathematics/Numerical Methods
Fellowship Years: 1997-2001
Current Status: Senior Scientist, General Electric

Ahmed Ismail
Massachusetts Institute of Technology
Molecular Simulations and Multiscale Modeling
Fellowship Years: 2000-2004
Current Status: Junior Professor, Mechanical Engineering, RWTH Aachen University

Amber Jackson
University of North Carolina
Applied Mathematics
Fellowship Years: 2004-2008
Current Status: Graduate Student

Nickolas Jovanovic
Yale University
Preconditioned Iterative Solution Techniques in Boundary Element Analysis
Fellowship Years: 1992-1994
Current Status: Founding Associate Professor of Systems Engineering, University of Arkansas at Little Rock

Yan Karklin
Carnegie Mellon University
Computational Neuroscience
Fellowship Years: 2002-2006
Current Status: Postdoctoral Researcher, Center for Neural Science/Howard Hughes Medical Institute, New York University

Richard Katz
Columbia University
Geodynamics, Coupled Fluid-Solid Dynamics
Fellowship Years: 2001-2005
Current Status: Academic Fellow, Department of Earth Science, University of Oxford

Benjamin Keen
University of Michigan
Conservation Laws in Complex Geometries
Fellowship Years: 2000-2004
Current Status: IDA Center for Computing Sciences

Peter Kekenes-Huskey
California Institute of Technology
Computational Chemistry and Biology
Fellowship Years: 2004-2007
Current Status: Postdoctoral Scholar, McCammon Group, University of California, San Diego

Jeremy Kepner
Princeton University
High-Performance Embedded Computing
Fellowship Years: 1993-1996
Current Status: Senior Technical Staff, MIT Lincoln Laboratory

David Ketcheson
University of Washington
Applied Mathematics: Numerical Analysis and Scientific Computing
Fellowship Years: 2006-2009
Current Status: Assistant Professor, King Abdullah University of Science and Technology

Sven Khatri
California Institute of Technology
Electrical Engineering
Fellowship Years: 1993-1996
Current Status: Honeywell Contractor

Jeffrey Kilpatrick
Rice University
Computer Science
Fellowship Years: 2008-2010
Current Status: Software Development Engineer, Microsoft

Benjamin Kirk
University of Texas
Aerospace Engineering
Fellowship Years: 2001-2004
Current Status: NASA Johnson Space Center

Bonnie Kirkpatrick
University of California, Berkeley
Computer Science
Fellowship Years: 2004-2008
Current Status: Graduate Student

Kevin Kohlstedt
Northwestern University
Coulomb Interactions in Soft Materials
Fellowship Years: 2005-2009
Current Status: Research Fellow, Chemical Engineering, University of Michigan

Justin Koo
University of Michigan
Electric Propulsion Modeling and Simulation
Fellowship Years: 2000-2004
Current Status: Engineer, Air Force Research Laboratory, Edwards Air Force Base

Michael Kowalok
University of Wisconsin
Monte Carlo Methods for Radiation Therapy Treatment Planning
Fellowship Years: 2000-2004
Current Status: Medical Physicist, Waukesha Memorial Hospital

Yury Krongauz
Northwestern University
Theoretical and Applied Mechanics
Fellowship Years: 1993-1996
Current Status: BlackRock

Eric Lee
Rutgers University
Mechanical Engineering
Fellowship Years: 1999-2003
Current Status: Engineer, Northrop Grumman Corporation

Miler Lee
University of Pennsylvania
Computational Biology, Developmental Genetics
Fellowship Years: 2005-2009
Current Status: Postdoctoral Associate, Yale University

Seung Lee
Massachusetts Institute of Technology
Computational Molecular Biology
Fellowship Years: 2001-2005
Current Status: Management Consultant, Boston Consulting Group (Seoul Office)

Jack Lemmon
Georgia Institute of Technology
Mechanical Engineering
Fellowship Years: 1991-1994
Current Status: Medtronic Inc.

Mary Ann Leung
University of Washington
Computational Physical Chemistry
Fellowship Years: 2001-2005
Current Status: Program Manager, Krell Institute

Brian Levine
Cornell University
Transport Systems
Fellowship Years: 2006-2010
Current Status: Graduate Student

Jeremy Lewi
Georgia Institute of Technology
Neuroengineering
Fellowship Years: 2005-2009
Current Status: Engineering Scientist, Intellisis

Benjamin Lewis
Massachusetts Institute of Technology
Computational Biology
Fellowship Years: 2002-2006

Lars Liden
Boston University
Educational Tools for Special Needs Children
Fellowship Years: 1994-1998
Current Status: Chief Technical Officer, TeachTown LLC; Software Technology Manager, University of Washington

Alex Lindblad
University of Washington
Computational Solid Mechanics
Fellowship Years: 2002-2006
Current Status: Senior Member of Technical Staff, Sandia National Laboratories – California

Tasha Lopez
University of California, Los Angeles
Chemical Engineering
Fellowship Years: 2000-2001
Current Status: Sales Specialist, IBM Cognos Business Analytics

Christie Lundy
Missouri University of Science and Technology
Physics
Fellowship Years: 1991-1994
Current Status: Missouri State Government

William Marganski
Boston University
Computational Biology, Imaging, Modeling
Fellowship Years: 1998-2002
Current Status: Research Scientist, Systems Biology Department, Harvard Medical School

David Markowitz
Princeton University
Computational Neurobiology
Fellowship Years: 2005-2009

Daniel Martin
University of California, Berkeley
Adaptive Mesh Refinement Algorithm and Software Development
Fellowship Years: 1993-1996
Current Status: Lawrence Berkeley National Laboratory

Marcus Martin
University of Minnesota
Monte Carlo Molecular Simulation (Algorithm Development Focus)
Fellowship Years: 1997-1999
Current Status: Director, Useful Bias Inc.

Randall McDermott
University of Utah
Numerical Methods for Large-Eddy Simulation of Turbulent Reacting Flows
Fellowship Years: 2001-2005
Current Status: Staff Scientist, National Institute of Standards and Technology (NIST)

Matthew McGrath
University of Minnesota
Computational Aerosol Physics
Fellowship Years: 2004-2007
Current Status: University Researcher, University of Helsinki (Finland)

Richard McLaughlin
Princeton University
Fluid Dynamics
Fellowship Years: 1991-1994
Current Status: Professor of Mathematics, University of North Carolina at Chapel Hill

Matthew McNenly
University of Michigan
Rarefied Gas Dynamics
Fellowship Years: 2001-2005
Current Status: Staff, Lawrence Livermore National Laboratory

Lisa Mesaros
University of Michigan
Aerospace Engineering and Scientific Computing
Fellowship Years: 1991-1995
Current Status: Business Manager, Fluent Inc.

Richard Mills
College of William and Mary
Scientific Computing
Fellowship Years: 2001-2004
Current Status: Computational Scientist, Oak Ridge National Laboratory

Julian Mintseris
Boston University
Computational Biology
Fellowship Years: 2001-2005
Current Status: Postdoctoral Fellow, Harvard Medical School

Erik Monsen
Stanford University
Entrepreneurship, Organization Development and Change
Fellowship Years: 1991-1993
Current Status: Senior Research Fellow, Max Planck Institute of Economics (Jena, Germany)

Brian Moore
North Carolina State University
Computational Simulation of Nuclear and Thermal-Hydraulic Processes in Boiling Water Nuclear Reactors
Fellowship Years: 1992-1995
Current Status: Leader, Methods and Software Development Center of Excellence, GE Hitachi Nuclear Energy

Nathaniel Morgan
Georgia Institute of Technology
Computational Fluid Dynamics
Fellowship Years: 2002-2005
Current Status: Los Alamos National Laboratory

James Morrow
Carnegie Mellon University
Sensor-Based Control of Robotic Systems
Fellowship Years: 1992-1995
Current Status: Principal Member of Technical Staff, Sandia National Laboratories – New Mexico

Sarah Moussa
University of California, Berkeley
Machine Learning and Genomics
Fellowship Years: 2003-2005
Current Status: Senior Software Engineer, Google Inc.

Michael Mysinger
Stanford University
Molecular Docking Solvation Models and G Protein-Coupled Receptor Docking
Fellowship Years: 1996-2000
Current Status: University of California, San Francisco

Heather Netzloff
Iowa State University
Quantum/Theoretical/Computational Chemistry
Fellowship Years: 2000-2004
Current Status: Community College Math Instructor and Tutor

Elijah Newren
University of Utah
Computational Biofluid Dynamics
Fellowship Years: 2001-2005
Current Status: Staff Member, Sandia National Laboratories – New Mexico

Pauline Ng
University of Washington
Computational Biology
Fellowship Years: 2000-2002
Current Status: Group Leader, Genome Institute of Singapore

Diem-Phuong Nguyen
University of Utah
Computational Fluid Dynamics (Combustion and Reaction)
Fellowship Years: 1999-2003
Current Status: Staff, University of Utah

Debra Nielsen
Colorado State University
Civil Engineering
Fellowship Years: 1992-1996

Oaz Nir
Massachusetts Institute of Technology
Computational Biology
Fellowship Years: 2006-2009

Joyce Noah-Vanhoucke
Stanford University
Fellowship Years: 2001-2003
Current Status: Scientist, Archimedes

Peter Norgaard
Princeton University
Computational Plasma Dynamics
Fellowship Years: 2005-2009
Current Status: Ph.D. (ABD) Candidate, Princeton University

Catherine Norman
Northwestern University
Computational Fluid Dynamics
Fellowship Years: 2000-2004
Current Status: Research Analyst, Center for Naval Analyses

Gregory Novak
University of California, Santa Cruz
Theoretical Astrophysics
Fellowship Years: 2002-2006
Current Status: Postdoctoral Fellow, Princeton University

Christopher Oehmen
University of Memphis/University of Tennessee Health Science Center
High-Performance Computing in Computational Biology
Fellowship Years: 1999-2003
Current Status: Senior Research Scientist, Computational Biology and Bioinformatics Group, Pacific Northwest National Laboratory

Steven Parker
University of Utah
Computational Science
Fellowship Years: 1994-1997
Current Status: Research Assistant Professor, Computer Science, University of Utah

Joel Parriott
University of Michigan
Elliptical Galaxies, Computational Fluid Dynamics, Parallel Computing
Fellowship Years: 1992-1996
Current Status: Program Examiner, Office of Management and Budget, Executive Office of the President

Ian Parrish
Princeton University
Computational Astrophysics
Fellowship Years: 2004-2007
Current Status: Einstein/Chandra Postdoctoral Fellow, University of California, Berkeley

Tod Pascal
California Institute of Technology
Physical Chemistry
Fellowship Years: 2003-2007

Virginia Pasour
North Carolina State University
Physical/Biological Modeling, Modeling of Epidemiological Dynamics
Fellowship Years: 1998-1999
Current Status: Program Manager, Biomathematics, Army Research Office

Christina Payne
Vanderbilt University
Molecular Dynamics Simulations
Fellowship Years: 2003-2007
Current Status: Postdoctoral Researcher, National Renewable Energy Laboratory

Chris Penland
Duke University
Computational and Statistical Modeling of Pharmacokinetic/Pharmacodynamic Systems for Biopharma
Fellowship Years: 1993-1997
Current Status: Expert Modeler, Pharmacometrics – Modeling and Simulation, Novartis Institutes for Biomedical Research

Carolyn Phillips
University of Michigan
Applied Physics
Fellowship Years: 2006-2010
Current Status: Graduate Student

James Phillips
University of Illinois at Urbana-Champaign
Parallel Molecular Dynamics Simulation of Large Biomolecular Systems
Fellowship Years: 1995-1999
Current Status: Senior Research Programmer, University of Illinois

Todd Postma
University of California, Berkeley
Nuclear Engineering, Computational Neutronics
Fellowship Years: 1994-1998
Current Status: Director of Engineering, Totality

David Potere
Princeton University
Demography/Remote Sensing
Fellowship Years: 2004-2008
Current Status: Consultant, Boston Consulting Group

Rick Propp
University of California, Berkeley
Computational Methods for Flow Through Porous Media
Fellowship Years: 1993-1996
Current Status: Senior Software Engineer, WorkDay

Alejandro Quezada
University of California, Berkeley
Geophysics
Fellowship Year: 1997

Catherine Quist
Cornell University
Bioinformatics
Fellowship Years: 2000-2004
Current Status: Postdoctoral Fellow, University of Michigan Cancer Center

Mala Radhakrishnan
Massachusetts Institute of Technology
Computational Drug and Biomolecular Design and Analysis
Fellowship Years: 2004-2007
Current Status: Assistant Professor of Chemistry, Wellesley College

Emma Rainey
California Institute of Technology
Planetary Sciences
Fellowship Years: 2003-2006
Current Status: Arete Associates

Nathan Rau
University of Illinois at Urbana-Champaign
Civil Engineering
Fellowship Years: 2000-2001
Current Status: Civil Engineer, Hanson Professional Services

Clifton Richardson
Cornell University
Physics
Fellowship Years: 1991-1995

Christopher Rinderspacher
University of Georgia
Inverse Design, Quantum Chemistry
Fellowship Years: 2001-2005
Current Status: Army Research Laboratory

John Rittner
Northwestern University
Grain Boundary Segregation
Fellowship Years: 1991-1995
Current Status: Chicago Board Options Exchange

Courtney Roby
University of Colorado
History of Science in the Ancient World
Fellowship Years: 2002-2003
Current Status: Assistant Professor, Cornell University

Alejandro Rodriguez
Massachusetts Institute of Technology
Nanophotonics, Casimir Effect
Fellowship Years: 2006-2010
Current Status: Postdoctoral Fellow, Harvard University

David Rogers
University of Cincinnati
Computational Physical Chemistry
Fellowship Years: 2006-2009
Current Status: Postdoctoral Research Fellow, Sandia National Laboratories – New Mexico

David Ropp
University of Arizona
Adaptive Radar Array Processing
Fellowship Years: 1992-1995
Current Status: Senior Scientist, SAIC

Robin Rosenfeld
Scripps Research Institute
Computational Biophysics
Fellowship Years: 1996-1997
Current Status: ActiveSight

Mark Rudner
Massachusetts Institute of Technology
Theoretical Condensed Matter Physics
Fellowship Years: 2003-2007
Current Status: Postdoctoral Fellow

Ariella Sasson
Rutgers University
Computational Biology and Molecular Biophysics
Fellowship Years: 2006-2010
Current Status: Bioinformatics Specialist, Children's Hospital of Philadelphia

David Schmidt
University of Illinois at Urbana-Champaign
Communications
Fellowship Years: 2002-2006
Current Status: Epic Systems

Samuel Schofield
University of Arizona
Computational Fluid Dynamics, Hydrodynamic Stability, Interface Methods
Fellowship Years: 2001-2005
Current Status: Scientist, T-5, Los Alamos National Laboratory

Christopher Schroeder
University of California, San Diego
Theoretical Particle Physics, Lattice Gauge Theory
Fellowship Years: 2005-2009
Current Status: Postdoctoral Researcher

Robert Sedgewick
University of California, Santa Barbara
Computational Biology
Fellowship Years: 2000-2003
Current Status: Research Associate, Carnegie Mellon University

Michael Sekora
Princeton University
Numerical Analysis, Godunov Methods, Multiscale Algorithms, Asymptotic Preserving Methods
Fellowship Years: 2006-2010
Current Status: Laurion Capital

Marc Serre
University of North Carolina
Environmental Stochastic Modeling and Mapping
Fellowship Years: 1996-1999
Current Status: Assistant Professor, University of North Carolina

Jason Sese
Stanford University
Hydrogen Storage on Carbon Nanotubes
Fellowship Years: 2003-2005
Current Status: Chemical Engineer, Environmental Consulting Company

Elsie Simpson Pierce
University of Illinois at Urbana-Champaign
Nuclear Engineering
Fellowship Years: 1991-1993
Current Status: Computer Scientist, Lawrence Livermore National Laboratory

Amoolya Singh
University of California, Berkeley
Dynamics and Evolution of Stress Response Networks
Fellowship Years: 2002-2006
Current Status: Scientist, Amyris Biotechnologies

Melinda Sirman
University of Texas
Engineering Mechanics
Fellowship Years: 1994-1996
Current Status: At Home

Benjamin Smith
Harvard University
Cloud and Mobile Computing
Fellowship Years: 2006-2010
Current Status: Software Engineer

Steven Smith
North Carolina State University
Chemical Engineering
Fellowship Years: 1992-1994
Current Status: Invista

Benjamin Sonday
Princeton University
Dimensionality Reduction/Computational Nonlinear Dynamics
Fellowship Years: 2006-2010
Current Status: Goldman Sachs

Eric Sorin
Stanford University
Simulational Studies of Biomolecular Assembly and Conformational Dynamics
Fellowship Years: 2002-2004
Current Status: Assistant Professor, California State University, Long Beach

Scott Stanley
University of California, San Diego
Large Scale Data Analysis, Search Engine Technology, Fluid Mechanics, Turbulence Modeling
Fellowship Year: 1994
Current Status: Vice President of Engineering, Buyful

Samuel Stechmann
New York University
Applied Math, Atmospheric Science
Fellowship Years: 2003-2007
Current Status: Assistant Professor, University of Wisconsin-Madison

James Strzelec
Stanford University
Computational Mathematics
Fellowship Years: 1992-1994

Rajeev Surati
Massachusetts Institute of Technology
Electrical Engineering and Computer Science
Fellowship Years: 1995-1997
Current Status: Scalable Display Technologies

Laura Swiler
Carnegie Mellon University
Reliability Analysis, Prognostics, Network Vulnerability Analysis, Combinatorial Optimization
Fellowship Years: 1992-1994
Current Status: Principal Member of Technical Staff, Sandia National Laboratories – New Mexico

Shilpa Talwar
Stanford University
Array Signal Processing
Fellowship Years: 1992-1994
Current Status: Senior Research Scientist, Intel Corporation

Brian Taylor
University of Illinois at Urbana-Champaign
Detonation, Shock Waves, Reacting Flow
Fellowship Years: 2003-2007
Current Status: National Research Council Postdoctoral Researcher, Naval Research Laboratory

Mayya Tokman
California Institute of Technology
Numerical Methods, Scientific Computing
Fellowship Years: 1996-2000
Current Status: Assistant Professor, University of California, Merced

William Triffo
Rice University
Biophysical Imaging, 3-D Electron Microscopy
Fellowship Years: 2003-2007
Current Status: Graduate Student

Mario Trujillo
University of Illinois at Urbana-Champaign
Two-Phase Flow, Computational Fluid Mechanics, Atomization Phenomena
Fellowship Years: 1997-2000
Current Status: Assistant Professor, Mechanical Engineering, University of Wisconsin-Madison

Obioma Uche
Princeton University
Molecular Simulation, Statistical Mechanics
Fellowship Years: 2002-2006
Current Status: Research Associate, University of Virginia, Charlottesville

Anton Van der Ven
Massachusetts Institute of Technology
First Principles Modeling of Thermodynamic and Kinetic Properties of Solids
Fellowship Years: 1996-2000
Current Status: Assistant Professor, Department of Materials Science, University of Michigan

Michael Veilleux
Cornell University
Computational Fracture Mechanics
Fellowship Years: 2004-2008
Current Status: Technical Staff Member, Sandia National Laboratories – California

Rajesh Venkataramani
Massachusetts Institute of Technology
Chemical Engineering
Fellowship Years: 1995-1999
Current Status: Goldman Sachs

Stephen Vinay III
Carnegie Mellon University
Application of Smoothed Particle Hydrodynamics to Problems in Fluid Mechanics
Fellowship Years: 1998-2000
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