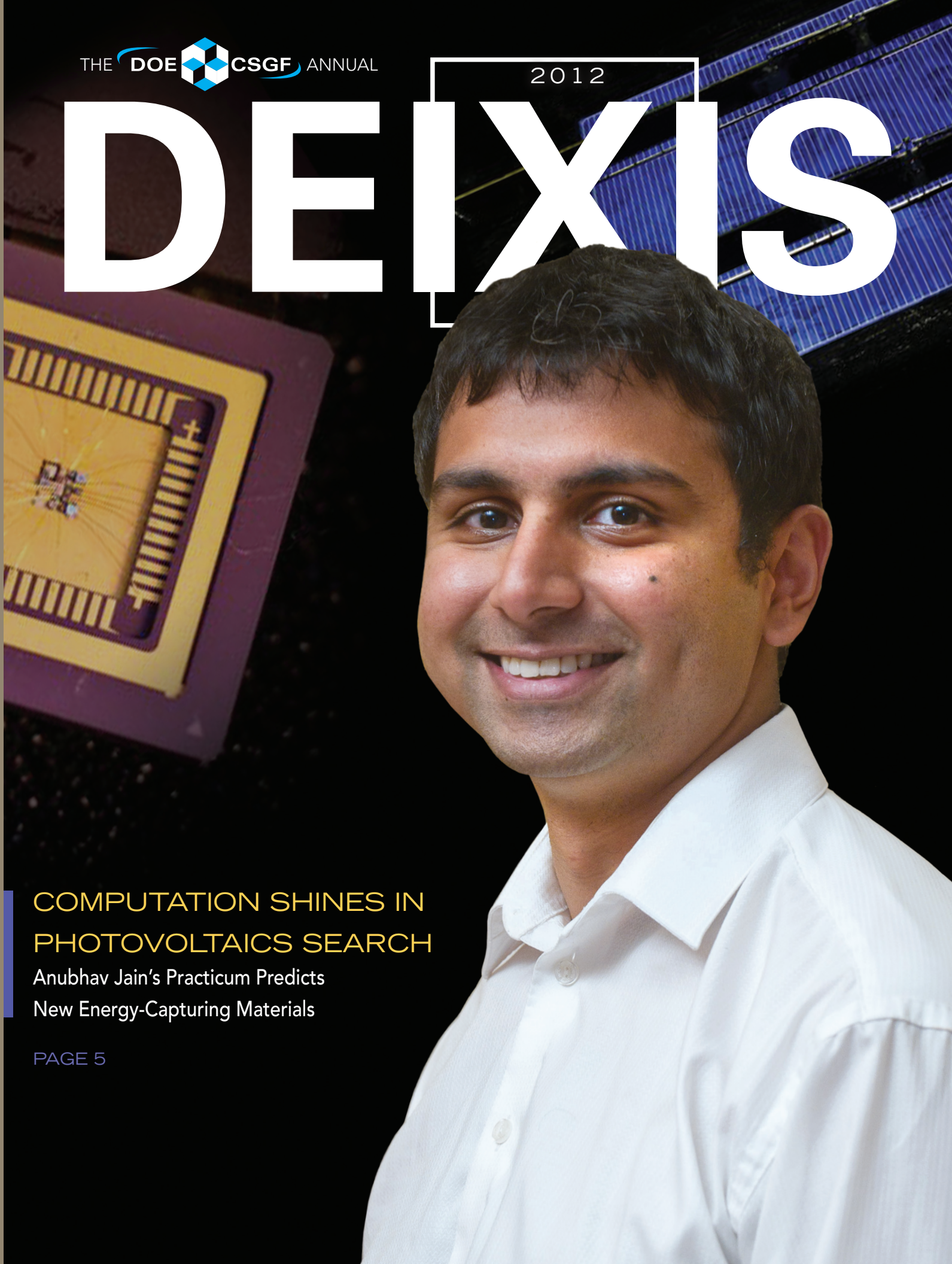
DEPARTMENT OF ENERGY COMPUTATIONAL SCIENCE GRADUATE FELLOWSHIP

THE DOE CSGF ANNUAL

2012

DEIXIS



COMPUTATION SHINES IN PHOTOVOLTAICS SEARCH

Anubhav Jain's Practicum Predicts New Energy-Capturing Materials

PAGE 5

THE DOE CSGF ANNUAL

DEIXIS

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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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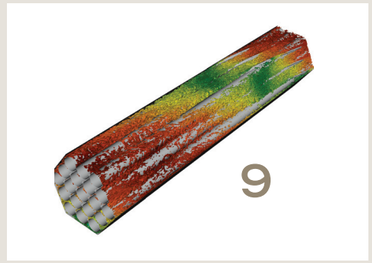
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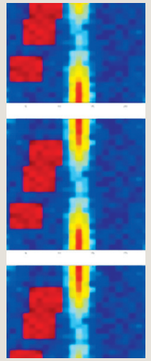
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PRIMED TO MEET PRIORITIES

The Department of Energy Computational Science Graduate Fellowship was established to train scientists who can apply the United States' growing computational power to important national needs, including those of the DOE. This issue of DEIXIS provides examples of how fellows and alumni do just that.

For example, the department emphasizes the rapid development of innovative materials for clean energy production and conservation. Fellow Anubhav Jain, profiled in this issue, helps drive that research with the Materials Project, a database of calculated compound properties.

The DOE CSGF also addresses the rising demand for scientists capable of implementing and using exascale computers – machines capable of a million trillion (10^{18}) calculations per second – expected to come on line later in this decade. Fellows Brian Lockwood and Hayes Stripling research uncertainty quantification, a key tool for maximizing exascale potential.

The fellowship meets these goals with a unique program that creates well-rounded students and exposes them to avenues outside their immediate field. This cross-pollination often results in surprising insights and lasting collaborations, as in the partnership of statistician Eric Chi and applied mathematician Tamara Kolda.

These are just a few examples of DOE CSGF fellows and alumni working to attack the issues facing us in the years ahead.

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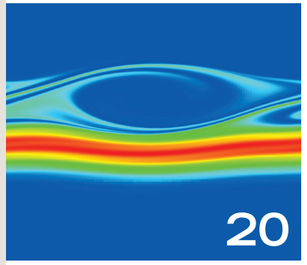
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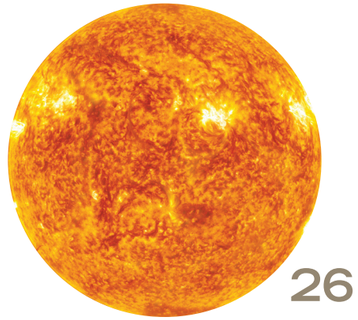
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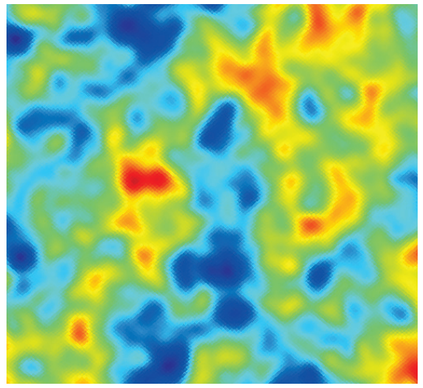
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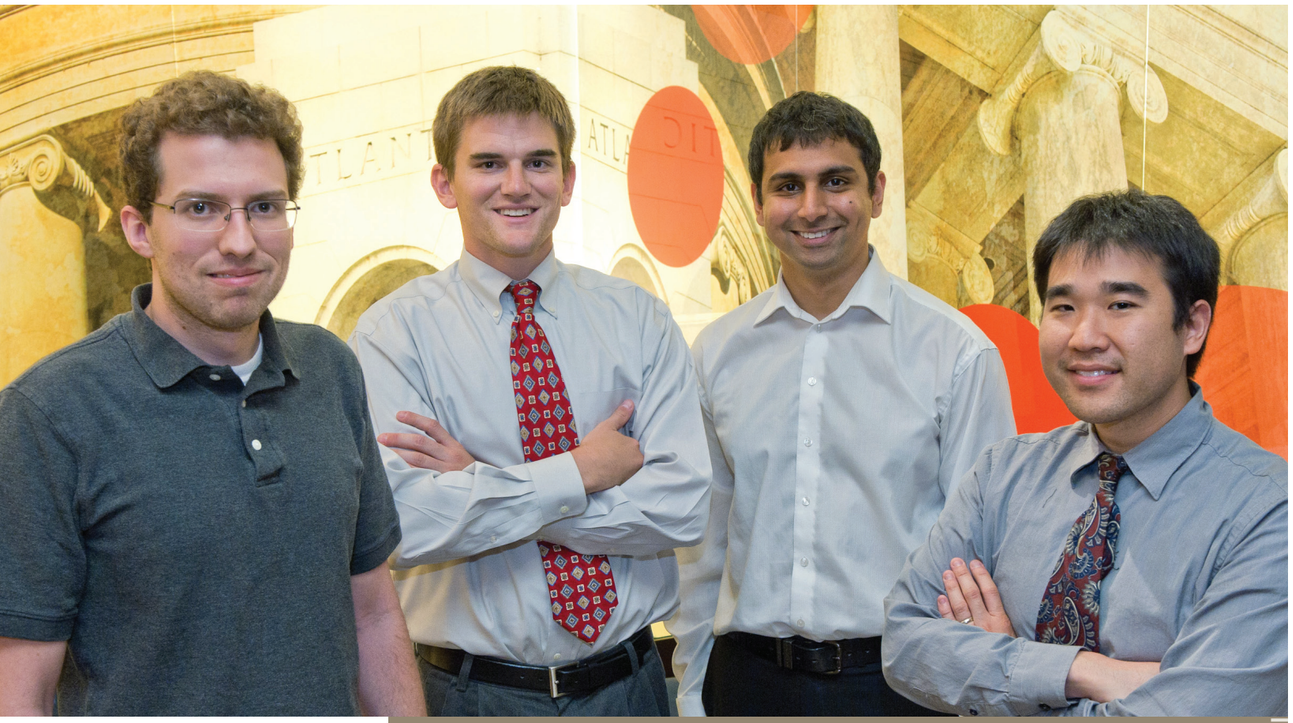
NOT YOUR USUAL SUMMER INTERNSHIP

LAB PRACTICUMS BRING FELLOWS PERSONAL AND PROFESSIONAL BENEFITS



Left to right:
Brian Lockwood, Hayes Stripling IV, Anubhav Jain and Eric Chi

IN THE CLASSIC CARICATURE of a summer internship, college students slave away at "gofer" duties and other tedious tasks.

Not so for Department of Energy Computational Science Graduate Fellowship recipients' summer practicums. Fellows are dispatched to national laboratories and tasked with hard problems – research subjects outside the bounds of the projects they carry out at their home universities. They work with leaders in subject matters of national importance and often employ some of the world's most powerful computers. The experience exposes fellows to the unique blend of resources and collaboration found at national laboratories.

The summer subject may be tangential to their doctoral project – like the materials research Anubhav Jain pursued or the uncertainty quantification projects Brian Lockwood and Hayes Stripling IV tackled. Or the summer may be a branch out into an interesting area outside their usual realm, as with Eric Chi's foray into tensor factorization. Either way, fellows return to campus with new perspectives and tools, both professional and personal.

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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RESEARCH COULD ILLUMINATE PROMISING PHOTOVOLTAICS

ANUBHAV JAIN
Massachusetts Institute of Technology
Lawrence Berkeley National Laboratory

WITH HIS FUTURE WIFE on the other side of the country during his summer 2010 practicum at Lawrence Berkeley National Laboratory (LBNL), Anubhav Jain had enough spare time to pick up a hobby.

The Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient bought a few books and dove into photography, testing his abilities with inexpensive digital cameras. The results are on his website, anubhavjain.net.

"I like composition a lot – how you can frame your shot so that things are at places your eye will be drawn to and how you can lead the viewer to certain things," says Jain, who earned his doctoral degree from the Massachusetts Institute of Technology (MIT) in August 2011.

Composition of a different type dominates Jain's working hours. He uses high-performance computers to calculate the properties of inorganic compounds of both untested and previously known compositions. The assessments portray a material's stability, energy-storing capacity and other qualities. Like a good photo, the calculations draw scientists' eyes to the most promising materials for synthesis and testing. The goal: Get new energy-saving and energy-producing materials to market faster.

Jain helped MIT Materials Science and Engineering Professor Gerbrand Ceder develop the Materials Genome Project, a computational encyclopedia of properties for inorganic materials. They combined powerful parallel-processing computers and density functional theory (DFT) algorithms to simultaneously portray the characteristics of tens of thousands of materials. DFT, a quantum mechanical modeling method, calculates the arrangement and interactions of electrons in atoms and molecules, breaking materials into geometrically arranged repeating cells to more easily capture the material's bulk properties. The problem, however, becomes more difficult as the number of electrons in each cell increases.

The Materials Genome has been used to predict material structures and screen for compounds suitable for purposes like absorbing mercury from coal gasification. With Ceder's group, Jain helped use its methods to computationally combine lithium with other elements in search of compounds for lighter, longer-lasting batteries. As a Luis W. Alvarez Fellow in Computational Science at LBNL, Jain now helps move the Materials Genome into its next iteration: the Materials Project.
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Jain's job was to find the simplest approximate approach that would make reasonable predictions about band gap and absorption spectrum.

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SWITCHING TO SOLAR MATERIALS

As with his MIT research, Jain's summer 2010 project goal was to devise high-throughput methods for computing the properties of thousands of new materials. This time he focused on identifying inorganic photovoltaic (PV) solids for solar power cells. If he succeeded, computers could rapidly screen compounds for their PV potential and find the most promising ones for testing. While they have huge potential for helping solve the world's energy problems, "it's just a lot harder to model solar PV properties than it is to model battery properties," Jain says. He worked with Jeffrey Neaton, director of the Nanostructured Materials Facility in LBNL's Molecular Foundry, which houses nanoscale theory, fabrication, testing and simulation research.

A compound's potential efficiency as a PV material depends, in part, on its ability to absorb sunlight, as represented by its absorption spectrum. The band gap is the minimum energy at which the material will absorb light, at the low-energy edge of this spectrum, liberating electrons from the array of atoms comprising it. Most photons in sunlight are in a tight range at relatively low photon energies – the visible spectrum. An ideal solar PV material has a band gap small enough to absorb those photons, but not so small that the electrons carry too little energy to do meaningful work. "What we really cared about," Jain says, "was how thick you need to make your solar cell material in order to absorb 85 percent of the incoming light. That's a function of the absorption spectrum."

As his baseline, Jain used calculations published in the journal *Environmental Science & Technology* in 2009 by Cyrus Wadia of the University of California, Berkeley, and collaborators. They combined band gap and absorption spectrum data with materials cost and availability information to compute several substances' potential for solar cell use. Interest in iron pyrite, commonly known as fool's gold, jumped when Wadia's group found it promising.

Wadia's team calculated solar PV feasibility for only 23 materials because they lacked band gap and absorption spectrum data for more. The challenge was to calculate those quantities for untested compounds, Jain says. "If we could do that, we could evaluate those materials' potential for use as next-generation solar PV materials."

KEEPING IT SIMPLE

There are considerable obstacles, however. The underlying DFT equations describing interactions between electrons and ions in atomic nuclei cannot be solved exactly, so DFT methods can find only approximate solutions. And while standard DFT methods do well calculating atoms and electrons in their low-energy ground state, they struggle to portray electrons that visible light has excited. Their ability to predict trends in band gaps is spotty.

Jain's job was to find the simplest approximate approach that would make reasonable predictions about band gap and absorption spectrum. The researchers wanted the computationally "cheapest and most meaningful predictive approximation we could make to give us some insight into what a new PV material would be," Neaton says. The simpler the approach, the easier it would be to scale up to rapidly assess hundreds of compounds.

Jain and Neaton compared two DFT methods that calculate how a material's energy changes as the electron charge density changes. The first, the generalized gradient approximation (GGA), is a standard approach that can have difficulty calculating the quantum mechanical property of electron exchange and correlation energy for certain materials. The second, HSE (named for the initials of its developers) is a hybrid, Neaton says, between a more computationally expensive, less approximate quantum mechanical approach and a standard approximation like GGA.

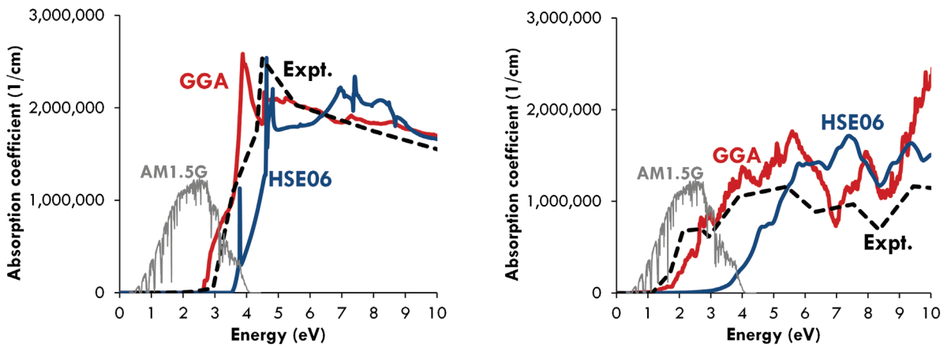
Jain ran GGA and HSE calculations for 17 materials in the Wadia paper – the ones for which he could find and digitize experimental data. GGA, as expected, failed to accurately calculate band gap or absorption for materials. HSE also gave imprecise solar PV property values, but produced trend lines that provided good predictions of practical quantities, like thickness, that the researchers sought. The low-level theories "were wrong in the fundamental quantity but then when you went up to the practical quantity they were OK," Jain says.

In the final analysis, some of the errors apparently cancelled: When Jain ranked 11 of the materials for solar cell suitability based on band gap and absorption spectrum, the projections matched four of Wadia's top five. "So it seemed like this method could actually be predictive" and scalable to screen thousands of materials, he adds.

More importantly, Neaton says, Jain made progress on developing a computationally inexpensive method to approximate solar PV properties in materials. "We brought the expertise on absorption and band gap calculations. He brought the tools to screen different compounds." Now that Jain's an LBNL postdoc, "We're very fortunate … because we can continue to work with him on that."

FOCUSING ON BATTERIES

The practicum gave Jain insights into leading-edge DFT methods and



These charts show the calculated and experimentally measured absorption coefficients of silicon (Si, at far left) and iron pyrite (FeS2, at near left). For reference, the solar spectrum is shown on an arbitrary scale and labeled "AM1.5G." For silicon, very little absorption occurs at energies overlapping with the solar spectrum. This is borne out in both GGA and HSE06 (hybrid) calculations. Typically, GGA redshifts the absorption spectrum compared to experiments, whereas HSE06 blueshifts, as is the case for silicon. Silicon's poor absorption is one of its major limitations as a photovoltaic material. In contrast, iron pyrite's absorption spectrum overlap with the solar spectrum is much greater, suggesting that much thinner films could be used to capture the same amount of light. This is correctly predicted by GGA calculations, particularly in the energy range relevant for solar capture (energies less than 4 electron volts). Somewhat surprisingly, iron pyrite's better absorptivity isn't reflected in HSE06 calculations. The behavior of iron pyrite as a solar cell material is indeed complex and poorly understood, and has been the subject of several detailed computational studies.
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PROJECT POOLS TALENTS FOR MATERIALS RESEARCH

The Materials Project, the next generation of the Materials Genome developed at the Massachusetts Institute of Technology (MIT), is more than a database of compounds' properties as computed and compiled on supercomputers.

It's also an arena for materials scientists, applied mathematicians and others to join forces on research into creating compounds key to clean energy, says Gerbrand Ceder, a professor of Materials Science and Engineering at MIT. "I know it all sounds very Zen-like, but it really is a much more collaborative platform" than the Materials Genome project he led. "We're making it easier for other researchers to come in with their skill sets."

The Materials Genome, which Department of Energy Computational Science Graduate Fellowship recipient Anubhav Jain helped establish, compiled huge quantities of computed materials property data. But, Ceder says, "our expertise was in phase stability and battery materials. We're now working in collaboration with other people who want to do this in, say, optimal properties of molecules for photovoltaics."

Computers based at Lawrence Berkeley National Laboratory's National Energy Research Scientific Computing Center host the Materials Project database. Along with machines at Berkeley Lab's Molecular Foundry and the University of Kentucky, NERSC also helps compute material properties like stability, voltage and capacity for dozens of new entries each day.

The database is expanding rapidly, Ceder says. As of May 2012, about seven months after launching, over 19,000 entries were online and more than 2,200 users had registered, about a quarter of them from industry.

excited-state calculations. He's hoping the Materials Project will hasten the search for promising solar cell materials.

The quest for new battery materials, meanwhile, has yielded results. While with the Ceder group, Jain helped sift thousands of lithium compounds, narrowing them down to one known and two previously unknown classes with promising characteristics. Ceder's group has submitted applications to patent the three compound classes for battery applications and is testing permutations of each. There's still a long road ahead, though, to test particle size, coatings and other characteristics before any could appear in batteries.

Jain was instrumental in developing the high-throughput system, Ceder says. "Nobody had ever built this in an automated way, that you could pull compounds out of a database and run the relevant calculations on them, store them in a database and systematically search that."

At LBNL, Jain is upgrading Materials Genome entries as they're moved into the Materials Project (*see sidebar*). The result should be more accurate computed values, Ceder says. "There's a higher level of scrutiny you need to apply" for a public database. "It's like the difference between cooking for yourself and opening up a restaurant. There's some difference in standards."

Jain wasn't unfamiliar with life at a lab before coming to LBNL. His father, Animesh Jain, is a physicist who brought his family, including 5-year-old Anubhav, to the United States from India when he joined Stony Brook University. The elder Jain later moved to DOE's Brookhaven National Laboratory on New York's Long Island. Nonetheless, Anubhav Jain says he's still uncertain whether he'll follow his father into the laboratory system. For now, he's content to work under a postdoctoral appointment before deciding whether to seek a permanent post or go into academia.

Neaton, for one, hopes Jain sticks around. "The work he's doing is in the spirit of a national lab. It's collaborative, it has a lot of relevance to some of the most important problems facing society in energy and other sectors. I think it's ideal for a lab setting."

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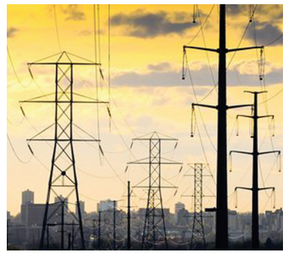
"Rapid uncertainty quantification techniques are core to how we make decisions every day," Lockwood says.



FELLOW PROBES PROBABILITY IN QUANTIFICATION QUEST

BRIAN LOCKWOOD
University of Wyoming
Argonne National Laboratory

IT'S AN UNCERTAIN WORLD. Everything from the weather forecast to the arrival time of our morning bus has an element of chance.

Yet, uncertainty rarely is at the top of our minds. "It's a matter of, 'Here are the handful of possibilities I can think of right now that I think are going to happen,'" says Brian Lockwood, a graduate of the Department of Energy Computational Science Graduate Fellowship (DOE CSGF). "And then, you think, 'All right, now I need to assign probabilities to those things.'" A rider catching the bus to work disregards the possibility a fly smashing into its windshield will delay it, but places more weight on a traffic jam holding it up. "Rapid uncertainty quantification techniques are core to how we make decisions every day," says Lockwood, who earned his doctoral degree earlier this year at the University of Wyoming.

Uncertainty quantification (UQ) is more difficult – but in many cases more vital – for computers simulating complex devices and processes. Uncertainty can arise from inexact experimental data, poorly understood properties of materials the models portray, imprecise calculations and other factors.

Take nuclear reactors, the subject of Lockwood's summer 2010 practicum at Argonne National Laboratory. Since building and testing reactors is prohibitively expensive, engineers use computer simulations to create and tweak designs that maximize fuel temperature for optimum energy production while still operating safely.

Those models are based on measurements of neutron transport cross sections, thermal conductivity and other inputs. But "what happens if my geometry is off by a little bit? Or my thermal conductivity that I measured in the lab – what happens if that's plus or minus 10 percent, and I happen to be toward the high side?" Lockwood asks. Engineers typically compensate for these doubts by building in huge margins of error – sometimes doubling the size or capacity of parts. It's like making a car twice as big or heavy as needed to ensure occupants' safety.

But engineers can begin to narrow that margin if computational scientists can put a number on the accuracy of a simulation's outputs. If thermal conductivity varies by 5 or 10 percent, computers can calculate how that affects the final outcome. "Instead of having to double everything, maybe I just add a margin of safety of 10 percent or 20 percent," Lockwood says. "All your designs, when you manufacture them, should be cheaper but should have the same level of reliability as when you over-engineered everything." Mihai Anitescu, a computational mathematician in Argonne's Laboratory for Advanced Numerical Software, says UQ gives policy-makers, engineers and scientists better information to make decisions or create designs.

In standard Monte Carlo UQ, researchers run thousands of random simulations with varying inputs to build probability curves describing the output's reliability. But today's complex models take days or weeks to run just once, making an ensemble of

UNCERTAINTY FOR EXASCALE COMPUTING

IF new reactors are to help revive the nuclear power industry, efficient ways must be found to calculate uncertainty inherent in the models used to design them, Mihai Anitescu says.

Anitescu, a computational mathematician at Argonne National Laboratory, heads uncertainty quantification research for CESAR, the Center for Exascale Simulation of Advanced Reactors. CESAR will mate multiphysics nuclear reactor simulation codes with exascale computers capable of a million trillion calculations per second – about a thousand times more powerful than today's best supercomputers. "My job is to put together advanced models for uncertainty and allow them to permeate to the next designs of reactors," Anitescu says.

During his summer 2010 practicum at Argonne, Department of Energy Computational Science Graduate Fellowship recipient Brian Lockwood helped Anitescu develop a way to incorporate gradient information into surrogate models used to calculate uncertainty. That method could help improve uncertainty quantification on exascale models.

"Anytime we talk about exascale, we're guessing big time. We're talking about a [computer] architecture no one has seen," Anitescu says. Yet he believes "decision-making under uncertainty has a computational pattern ideally suited for exascale."

To be energy efficient, any exascale computer will need to perform lots of floating point operations for every time processors communicate or access memory. "Uncertainty analysis tends to deliver that," Anitescu adds. "On top of that, decision-making under uncertainty has a computational pattern which is very suitable to that, yet … can't be achieved" with today's computers.

calculations prohibitively expensive, in computational terms. Working with Anitescu, Lockwood tackled the problem of getting useful uncertainty quantification with a limited number of simulation runs.

Their approach: build simple, less demanding surrogate models "trained" on data from the full simulations. Researchers can run a surrogate thousands of times to predict uncertainty in outputs from the full, baseline model. But a surrogate's usefulness depends on how it's constructed. One that makes good assumptions about data between points obtained from the full model often is more precise, even if information from the full model is sparse.

"You can get pretty good estimates of your statistics with relatively low error, simply because you constrain what the model is going to look like between sample points," Lockwood adds. He and Anitescu developed "what we think is a pretty good way to combine those samples in a smart way, utilizing a few things you know about the problem in order to get really good statistics on your output with only a handful of baseline simulations."

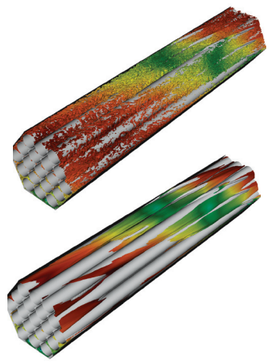
CLIMBING A GRADIENT

Their approach, GEUK, for gradient-enhanced universal Kriging (pronounced *kreeging*), built on Anitescu's research incorporating gradient information into polynomial regression surrogate techniques.

"Regression models tend to be superficial in terms of how they assume the error to behave," Anitescu says. GEUK can reduce uncertainty and is more general, so that slight changes in the problem don't lead to substantially different uncertainty predictions.

In essence, the GEUK surrogate combines training data from the full model with gradient data representing how much an output changes in response to an input change. In a sense, gradients tell researchers something about the shape of the simulation's design space – the outputs possible for a set of parameters. Gradients are a derivative, which describes the rate of change in a quantity with respect to another quantity. For example, velocity is a derivative of the distance an object travels over time.

It costs relatively little additional computer time for the full-size simulation to calculate derivatives at the same time it generates outputs, Lockwood says, yet incorporating gradients further constrains the surrogate. "If I put more constraints on what my model needs to look like as I go through the points I've actually sampled, I get a higher-quality surrogate."

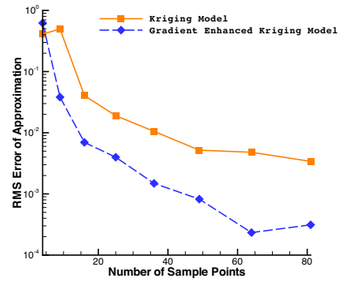


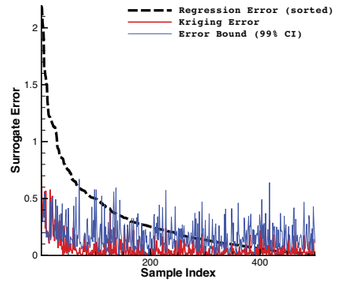
These visualizations show simulations of isosurfaces of axial flow velocity in a 19-pin nuclear fuel rod bundle with wire-wrap spacers. Color indicates the variation in pressure (blue-green is low, orange-red is high) as coolant moves through the bundle. The upper image shows an instantaneous snapshot of the turbulent flow field. The lower image shows the time-averaged field. The simulations were performed with 360,000 spectral elements of order N=7 (123 million grid points) on the IBM Blue Gene/P at the Argonne Leadership Computing Facility.

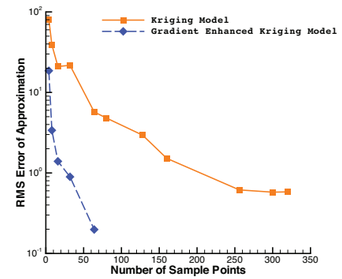
Top right: Comparison of Kriging error in approximating the cosine function. Incorporating gradient information into the Kriging model decreases the number of samples required for an accurate approximation.

Middle right: Point-wise error comparison for approximating the output of a MATLAB thermohydraulics model. The simulation output for a variety of inputs can be accurately predicted using only eight simulation results and associated gradients.

Bottom right: Global error comparison for predicting the MATLAB thermohydraulics model output. When gradients are incorporated into the Kriging model, the number of baseline simulations required for an accurate surrogate is greatly diminished, allowing for uncertainty quantification within an affordable budget.







The final element in Lockwood's approach is Kriging, which considers the distance between points when deciding how much they're correlated and how much weight to give them when estimating the location of an unknown point.

Kriging flexibly incorporates gradients in the surrogate, Lockwood says. It also addresses bias in standard regression techniques, meaning the predictions they generate may not intersect all the training data points. "That's not a great thing to have in a surrogate," Lockwood says. "Kriging ensures my surrogate matches at every single point that I sampled" in the full model.

Universal Kriging not only provides a mean prediction for each sample, but also estimates its variance. A large variance means the surrogate doesn't have enough data from the full model to make a good prediction. Either more sample data are needed or the surrogate's predictions must account for the variance.

"You have uncertainty due to input parameters and you also have uncertainty based on your surrogate model," Lockwood says. Kriging "allows you to easily assign confidence even on the surrogate prediction itself."

To test the GEUK method, Lockwood and Anitescu ran a simplified nuclear reactor model hundreds of times with varying input parameters to generate a database of peak fuel pin temperature predictions. They trained the surrogate with a small set of data points and derivatives obtained from the model.

To assess accuracy, the researchers probed the surrogate and compared the results with those the full model generated. Even with as few as eight training points the surrogate approximated the full model's behavior with errors of less than 1 percent, Lockwood says.

Lockwood and Anitescu published a paper on the research in a recent issue of the Journal *Nuclear Science and Engineering* [1]. Lockwood also presented at the 2011 Society for Industrial and Applied Mathematics Conference on Computational Science and Engineering and the American Nuclear Society 2011 annual meeting. Lockwood, Anitescu and Lockwood's doctoral advisor, Dimitri Mavriplis, also submitted a paper for a meeting of the American Institute of Aeronautics and Astronautics in January 2012, calculating the effects of uncertainty arising from the combination of random circumstances and imprecise measurements. Anitescu, meanwhile, will include GEUK in a software "toolbox" for surrogate model construction.

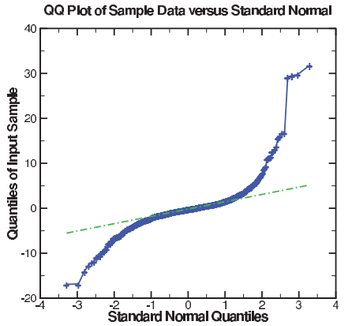
GOING HYPERSONIC

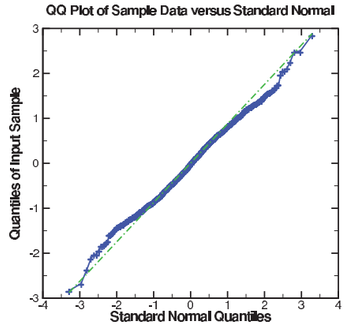
Lockwood embraced GEUK's Kriging component for his doctoral research on modeling hypersonic flows – those moving at speeds of at least Mach 5, such as those spacecraft encounter when returning to earth.

"The two things you need to know about hypersonic flows are they're really, really hard to solve and they're really, really nonlinear," Lockwood adds. That means looking at one point in a distribution or at data from a specific location tells researchers little about what will happen overall.

Lockwood and Mavriplis, a mechanical engineering professor at Wyoming, used adjoint techniques to solve hypersonic flows with sensitivity analysis – assessing which input parameters most influence a particular simulation output. Derivatives are key to sensitivity analysis, but the standard approach of linearizing equations, then solving them and calculating derivatives, requires deciphering a different problem for each of perhaps hundreds of inputs.

[1] Lockwood, Brian A., and Anitescu, Mihai, "Gradient-Enhanced Universal Kriging for Uncertainty Propagation," *Nuclear Science and Engineering*, Vol. 170, No.2, February 2012, pp. 168-195.





Distribution of error associated with Kriging predictions using eight (near right) and 50 (far right) baseline solutions. Due to the nature of Kriging models, uncertainty in predictions can be calculated, allowing researchers to associate a confidence level with their predictions.

An adjoint method, in contrast, transposes the linearized equations. "Instead of sweeping through them forward, I sweep through them backward," Lockwood says. "This variable pops out, called the adjoint" that can quickly calculate a single output's sensitivity to multiple inputs. Once calculated, the uncertainty inherent in each input can be propagated through the model and weighted by the output's sensitivity to them.

"My contribution," Lockwood says, "has been computing gradients on these hypersonic flows, something I haven't seen many other people do." Lockwood upped the degree of difficulty, Mavriplis says, by calculating sensitivity analysis and uncertainty quantification on flows involving reacting gases. That "opens up a whole new ballgame, where you have all these model parameters – real gas reaction rates and transport coefficients that all have inherent uncertainties associated with them."

Kriging uses sensitivity analysis data to handle the nonlinear nature of parameters affecting a simulation's output. Lockwood had used a Kriging code before his practicum, but had only a vague notion of how it worked. Now he's replaced the group's Kriging code with his Argonne method. "I've gone from being one of the users of Kriging in my lab to being the expert on it."

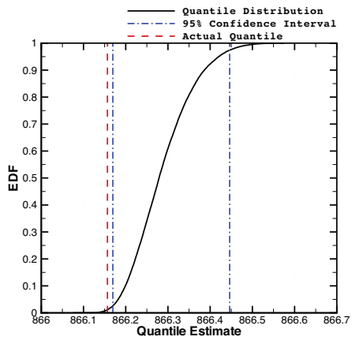
Not bad for someone who says the practicum got him into "some of the math that normally makes my eyes gloss over. It gave me more confidence to tackle these more purely mathematical problems."

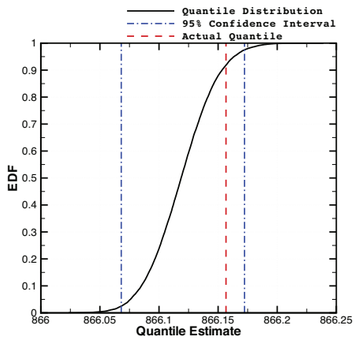
It was just a matter of picking the right problem, Anitescu says. Lockwood is "really an extraordinary engineer, so we went for something that was extensive, not intensive." Finding the best Kriging approach requires "quite a bit of empirical work, albeit mathematical empirical work. That's very suitable for an engineer."

Lockwood, a Georgia native who earned a nuclear engineering master's degree at the Georgia Institute of Technology, interned for two summers at the Idaho National Laboratory and came to Wyoming after colleagues recommended Mavriplis, a top computational fluid dynamics researcher. "I wanted to be treated more as a collaborator as opposed to someone trying to mentor me," Lockwood says, and Mavriplis fit the bill.

It's been a profitable collaboration, Mavriplis says. Lockwood "really understands the material and he's meticulous about it. He's also interested in pursuing it until he implements it – or reimplements it" – for his own purposes. DOE CSGF alumni are "highly sought after, so I think he could go to any of the labs."

Anitescu agrees. Lockwood "enjoys interdisciplinary experiences. We badly need people like him in the lab system."





Prediction of the 99th percentile using eight (far left) and 50 (near left) baseline solutions. Because Kriging is statistical in nature, the predictions are given by a continuum of values with associated probabilities, allowing researchers to specify relevant statistics and the amount of confidence in the prediction.

MOVIE CHALLENGE SPARKS PRACTICUM – AND A SEQUEL

ERIC CHI
Rice University
Sandia National Laboratories – California

APPLIED MATHEMATICIAN TAMARA KOLDA says she hadn't even considered recruiting a statistician for a practicum before Eric Chi contacted her. "That was completely naïve and foolish," she says now. "I didn't know I needed to meet him or someone like him."

Chi, meanwhile, had done a practicum at Lawrence Berkeley National Laboratory for his Department of Energy Computational Science Graduate Fellowship (DOE CSGF). It was a good experience, but he wasn't considering another.

Netflix brought Chi and Kolda together, leading to 2010 and 2011 practicums and an intersection of interests that's generated new ways to identify patterns in sparse data, like email correspondence or blurry medical images.

Chi was intrigued by the Netflix Prize, the online video rental company's million-dollar offer to anyone who could improve the performance of its movie recommendation algorithm by 10 percent. To the layman, that sounds like a scant gain, but after almost three years the winning team of mathematicians and statisticians eked out just a 10.06 percent improvement.

To train their algorithms, Netflix Prize teams used a database of almost 100.5 million ratings of 17,770 movies posted by 480,189 customers. That information can be displayed as a matrix – a table with customers along the left edge and movies across the top. With more than 8 billion possible combinations of movies and customers, the fact only 100 million ratings are filled in means most of the table's cells are empty, says Chi, who earned his doctorate in statistics from Rice University last summer. With so little data for analysis, "it looks like a completely impossible task to make decent predictions," he adds. "But it's not impossible to have some improvement."

Scientists often face a similar problem. Experimental or observational data are sparse when equipment fails or a response is weak. Researchers need good statistical methods to draw accurate conclusions. The key is finding patterns – the systematic variation – and what generates them amid non-systematic variation – the random data commonly called noise. It's like separating wheat from chaff, Chi says.

"It looks like a completely impossible task to make decent predictions," Chi adds. "But it's not impossible to have some improvement."

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TURNING TO TENSORS

Chi was pondering the Netflix Prize in late 2009 when he met Kolda at a DOE gathering. Kolda, a distinguished member of the technical staff at Sandia National Laboratories' Livermore, Calif., campus, specializes in developing methods to analyze tensor data.
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"I saw this great opportunity to branch out into an area I wasn't doing before."

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Tensors characterize data that have multiple dimensions. Netflix data are indexed in two dimensions, but "there's lots of data out there that can be indexed three, four, five – whatever ways," Chi says. Video images can be three-dimensional tensors: each pixel in a frame is indexed on X or Y axes and in time. In brain imaging, tensor data can include time, frequency, experimental conditions and other dimensions.

"Tammy was doing these tensor models and I thought, 'Oh, they're actually very similar to this Netflix data,'" Chi says. "I saw this great opportunity to branch out into an area I wasn't doing before."

Like the Netflix Prize, Kolda's work deals with sparse data and factorization, also known as decomposition, which produces a simpler picture of a matrix, making it easier to analyze or perform computations on its data. Tensor factorization is similar, but with multiple dimensions.

Kolda and Chi focused on alternative ways to account for error when fitting mathematical models of patterns – the systematic variation – with data to judge the model's accuracy. "You need some measure of goodness of fit," called the loss, Chi says. Data-fitting techniques often make assumptions about nonsystematic variation – the chaff. If it doesn't behave as expected, it will be hard to accurately separate it from the wheat – the systematic variation.

Chi's approach discarded standard "least squares" error measurement in favor of a "least 1-norm" approach that copes better with noise outside a Gaussian, or bell-shaped, curve. (*See sidebar, page 16.*) It was interesting work, Kolda says, "but what was more interesting, at least for me, was the idea you should even think outside of least squares error." Chi "changed my view of the world, and that's unusual. He really opened up questions and ideas that were new to me."

EMAIL ANALYSIS

In summer 2011 Chi's goal was again to find factors generating patterns in sparse data, but with some differences: The data were based on counts of things, like interactions between two or more parties; and they're nonnegative, so each count is zero or more.

For instance, researchers may want to study email correspondence to predict who will email whom, when and how often. "If you look at, say, a group of 100 people, they're not all emailing each other," Kolda adds. But "maybe there are subgroups that are emailing each other quite a bit," so the data are sparse.

Most transactional data, like phone calls, purchases or network traffic, has this sparse count structure, Kolda says, so the technique she and Chi developed could have applications in national security, marketing, network administration and even modeling social networks. "The simple latent picture you're trying to suss out is community structure," Chi says.

Chi borrowed a familiar technique: maximum likelihood estimation (MLE) with an assumed Poisson data distribution, which typically describes counts of independent events over time. The MLE finds model parameters under which observations are most likely. The technique, called CPAPR (CANDECOMP/PARAFAC alternating Poisson regression) "gives a nice, succinct summary for how different trends in each of different measurement modes are interacting to generate the data," Chi says.

Chi and Kolda tested the method on at least two data sets, including email from Enron, the energy trading company that crashed in 2001 amid a Securities and Exchange Commission (SEC) investigation into financial misdeeds. The tensor data had three dimensions: sender, receiver and time. The researchers also had information about correspondents' jobs and departments.

"The cool thing about this model is, for the tensor factorization, it automatically sorts out the sender and receiver groups over time," Chi adds. "You'll see (members of) the legal department talking with other members at X number of days before the SEC investigation and things like that."

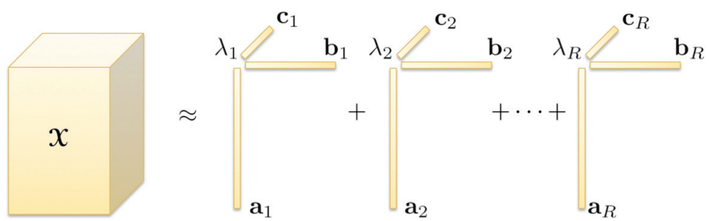
Chi and Kolda have submitted a paper detailing their results.

Like his 2011 Sandia project, Chi's doctoral research dealt with sifting through noise, outliers and other problems to find patterns in complex, high-dimensional data with sparse samples of real data points. He and advisor David Scott researched approaches that could be useful to screen gene expression data and find effective disease treatments. With huge yet sparse bioinformatics datasets, "it's becoming less and less practical to invest time cleaning up the data before you do your analysis," says Scott, the Noah Harding professor of statistics at Rice. The algorithms his group develops simultaneously propose models and analyze their fit.

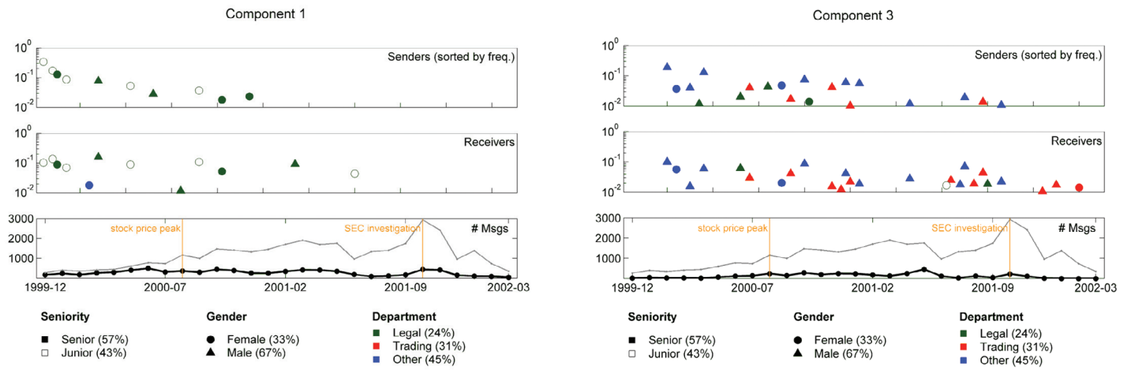
"There are two strategies: I want to reduce error overall, or I can tolerate some really bad errors if the less-bad errors are super, super small," Chi says. MLE takes the first approach, making it sensitive to large errors. Scott says the integrated square error approach he calls L2E does the latter. "If there's a bad data point you're not going to make it go to zero. You … sort of tag it as something that doesn't fit the model."

Chi and Scott performed tests showing the method handles contamination better and copes with misspecification: choosing the wrong modeling method because of faulty data assumptions. "If you start with a model that's too simple, then usually the estimation is pretty messed up," Scott says. With L2E, "if the model you specify is appropriate for a subset of the data … it can find that subset and model it. Then it will indicate which data points it's not trying to model."

Scott says Chi's thesis research and practicums overlapped slightly, but Chi mainly benefitted from working in a different discipline. As one of the few statisticians at Sandia, Chi "really came away with some perspective about how to talk about the nonstatistical things with very smart scientists."



The CP (CANDECOMP/PARAFAC) model approximates a tensor, x, with a linear combination of rank-1 tensors. In the figure, λ_i is the weight controlling the contribution of the *ith* rank-1 tensor to the approximation, and the *ith* rank-1 tensor is the outer product of the three vectors a_i, b_i and c_i.



The components capture email conversations between different Enron Corp. groups at different times. The first row in each subfigure tracks the outbound email activity of certain employees, the second row the inbound email activity of particular employees and the heavy dotted line in the third row the total number of messages due to the component under consideration. For reference, the time mode is annotated by the time at which Enron's stock price peaked and when the SEC investigation began. The light gray line shows the total message volume. It is interesting to observe how the components break down into specific subgroups. For instance, Component 1 consists almost entirely of legal department employees and is majority female. This can be contrasted to Component 3, which tracks conversations among senior employees, most of whom are male, in departments other than trading and legal. Note that the algorithm separated out these components without knowing the rank, gender or department of the employees.
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TURNING DOWN THE NOISE IN DATA

When fitting mathematical models of patterns to existing data, what researchers believe about noise makes a big difference, Eric Chi says.

The least squares method commonly used to calculate loss in tensor-based models assumes noise is Gaussian – distributed in a bell-shaped curve. That's usually a good assumption, Chi says, but there could be non-Gaussian variations. Surveillance videos, for instance, change little from frame to frame, but an object or person crossing the picture produces the high intensity, sparse noise least squares is sensitive to, potentially disrupting the method.

The least 1-norm approach Chi used in his 2010 practicum is "willing to have one or two large errors if it can shrink a lot of smaller errors down to zero." But the approach is more difficult to solve, so Chi tapped a majorization-minimization algorithm that takes an indirect approach to shrink small errors and breaks the problem into easier steps.

Chi tested his algorithm, named CPAL1 (CANDECOMP/PARAFAC alternating least 1-norm) on data designed to emulate video surveillance footage: a 256-pixel square image of a blue and red blob changing shape over 200 time steps. First Gaussian noise, resembling snow, obscured the image. The standard least squares algorithm picked out the image perfectly. CPAL1 did nearly as well.

Next, Chi seeded the image with both Gaussian "snow" and random blotches of irregular noise. CPALS produced a blob bearing little resemblance to the true image. CPAL1, however, reproduced it nearly perfectly.

Chi and Kolda produced a technical report on the project and Chi presented the research at a lab seminar and at the 2010 Neural Information Processing Systems Foundation workshop.

Kolda agrees. "I loved that (Chi) was interested and open not only to learning what I knew but teaching me about what he knew – with a lot of patience."

Chi praises Kolda as both a researcher and a mentor. "It's just awesome to be able to work with the 'queen of tensors' from the applied math community," he says.

"I think it would be very foolish not to build on it" with further collaboration.

Of course, Chi must fit that in around his postdoctoral position at the University of California, Los Angeles, under Kenneth Lange, where he's still seeking signals in complex data – DNA sequences – and, in the long run, a faculty post.

"I loved that (Chi) was interested and open not only to learning what I knew but teaching me about what he knew – with a lot of patience."

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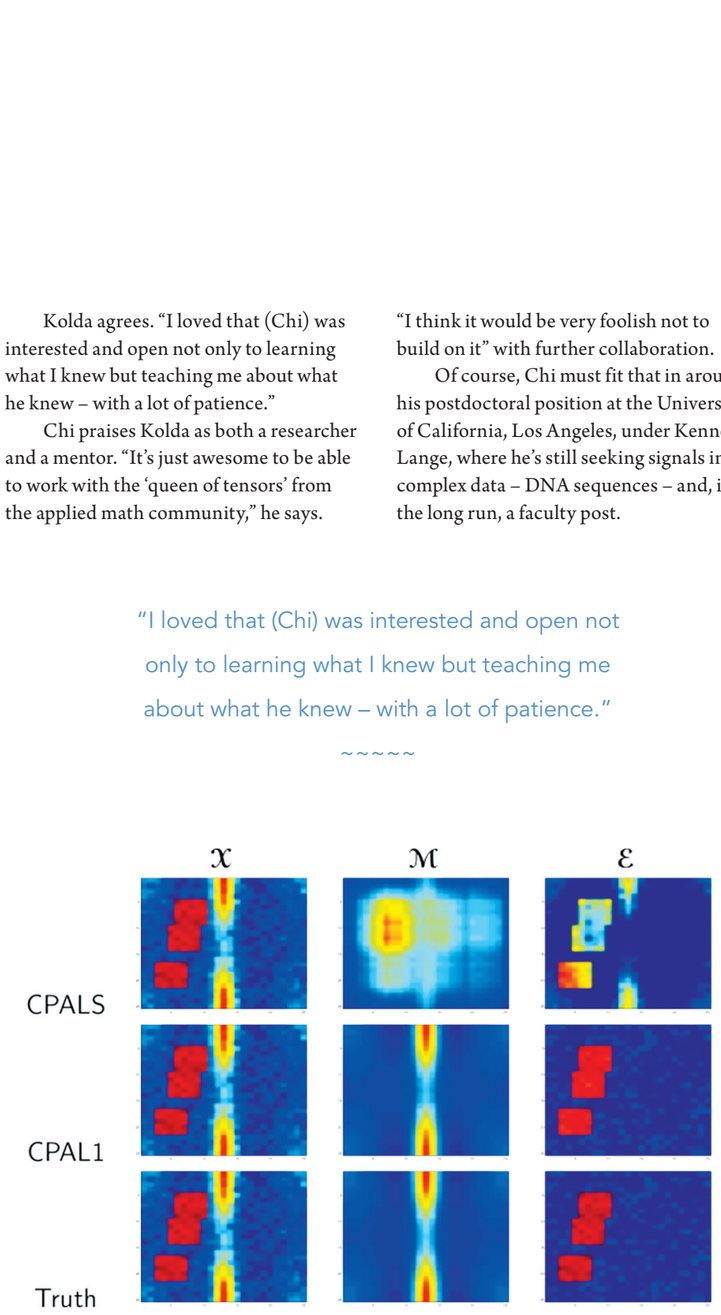

The first two rows show the results of separating Gaussian and non-Gaussian noise from low rank 3-way data by CPALS and CPAL1 respectively. The last row shows the underlying true decomposition. The left column shows observed data. The middle column shows the recovered low-rank structure. The right column shows the residual error.

Many of the tools and skills he's applied were collected during practicums arranged at national laboratories under his Department of Energy Computational Science Graduate Fellowship.

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SAMPLING SURROGATES TO WEIGH UNCERTAINTY

HAYES STRIPLING IV
Texas A&M University
Lawrence Livermore National Laboratory

IN HIS FORMATIVE YEARS, Hayes Stripling IV spent weeks hunting quail and doves in the scrub near Big Spring, the west Texas town where the three previous Hayes Striplings grew up.

Now, Stripling zeroes in on something much different: uncertainties in computer simulations. Uncertainty quantification (UQ) is a rising research area that puts a number on the amount of error in results from complex computer models. That error may come from imprecise input data, characterizations of unmeasurable physical processes, rounding numbers in calculations and other sources. UQ gives scientists and policy-makers an idea of how reliable computer predictions are.

As a nuclear engineering doctoral student at Texas A&M University, Stripling has become adept at targeting uncertainty. Many of the tools and skills he's applied were collected during practicums arranged at national laboratories under his Department of Energy Computational Science Graduate Fellowship (DOE CSGF).

In 2010, Stripling worked under Gardar Johannesson, a senior applied statistician at Lawrence Livermore National Laboratory, and tied into the UQ Strategic Initiative, the lab's interdisciplinary effort to refine UQ methods. Johannesson focuses on UQ methods to automate the way inputs to simulations are chosen and calibrated to more accurately predict reality.

Today's detailed models of complex processes like nuclear reactor operation and climate evolution can take weeks to run, even on powerful computers. Only a few runs are possible – "far fewer than you would actually like to do," Johannesson says – each with slightly different uncertain inputs to build a database of results. That's used to train a statistical response model that tries to accurately predict results the full-scale code would produce given a set of previously untried inputs. Response models also help focus on the most important parameters, addressing the dreaded curse of dimensionality: The number of possible combinations to explore grows exponentially with the number of inputs that can influence the results. Climate models, like the Community Atmospheric Model (CAM) the Livermore researchers use as a test bed, are "the epitome of the curse of dimensionality," Stripling adds.

Statistical response models are, essentially, surrogates for the full simulation – simpler versions researchers can quickly sample thousands of times, tweaking the inputs each time to calibrate them to the full model and produce results for UQ. They infer the mapping between a simulation's inputs and outputs: If a set of 10 inputs leads to a set of 10 outputs in the full simulation, the response model builds a mathematical function that replicates the results. "If I want to get an idea for what my big simulation would give me at a new set of inputs – an 11th input set, if you will – then this response model should give me a good guess but at a very cheap cost" in computer time, Stripling says. "Even more importantly, the response surface should give me an idea as to how confident it is in that prediction," thereby quantifying uncertainty.

"The sky's the limit for Hayes," says Adams, a professor of nuclear engineering. "He's exceptional."

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But, Johannesson says, using a surrogate "adds uncertainty to the whole thing. It's just a statistical model that's trained on data from the code." In his practicum, Stripling focused on accounting for that added uncertainty, something not routinely done in previous research. His goal, Johannesson says, was "to look into a particular new method that has been proposed. We wanted to learn more about it so it was a perfect opportunity for him to dive into that."

GOING TO MARS

The method starts with Multivariate Adaptive Regression Splines (MARS), which generates "splines" – simple mathematical representations of possible responses to varying inputs. The method creates several candidate splines, then looks for ones that fit the training data in the simplest and most accurate way.

To incorporate the response model's inherent uncertainty, Stripling added a new twist: a Bayesian approach (Bayesian Multivariate Adaptive Regression Splines or BMARS) that samples an ensemble of MARS models instead of one. "Say we have a set of five inputs that can vary between a low value and a high value. We just pick a point randomly in that input space and use BMARS to predict what the climate model would give us," Stripling says. The algorithm compares the prediction with real-world data and evaluates the likelihood that set of inputs accurately depicts reality. It accepts or rejects the proposed point and moves to another one. "At the end of the day you have this group of points that have been accepted. That's how you form a probability space on the inputs." The technique also helps tackle dimensionality because "the BMARS surrogate will zero in on the important parameters," Stripling says.

To test the algorithm, Stripling targeted a specific CAM output: long-wave radiation flux, also known as FLUT, a measure of the energy Earth's surface reflects back into space. He trained the BMARS model on data from 714 runs of the full model, then sampled outputs from the simplified model. The approach improved the distribution of FLUT outputs from multiple model runs. "If that distribution is extremely wide, in some sense, and flat, that means we don't know much about that output," Stripling says. A narrow distribution indicates "we're zeroing in on some answer, which is the average of that distribution that we're starting to have some confidence in." BMARS also ensured the center of the narrower distribution falls on a data point from real-world measurements.

Using BMARS, Stripling worked with 21 inputs – from among hundreds of possibilities – that drive FLUT the most, then calibrated them and ranked them in order of importance. "We were able to zero in on what the actual values of the uncertain inputs are that are making our simulation more accurate. And then we were also able to improve that output distribution and move it toward the satellite data."

Stripling presented a poster on the project at Livermore's summer intern symposium and earned a prize for the best student poster from the computation directorate. He also presented the research in a lab seminar. Since then, Johannesson says his group has reimplemented the approach in a UQ code to analyze multiple response models.

The practicum, Stripling says, "opened doors and put new tricks in my bag of tricks, as my advisor (A&M's Marvin Adams) likes to say. It's given me the opportunity to become not an expert, but a more informed person on some of these broader fields."

Stripling pulled out one of those tricks to help with a project involving experiments conducted by the Center for Radiative Shock Hydrodynamics (CRASH), a collaboration involving A&M and the University of Michigan. Using powerful laser pulses, CRASH researchers drive a beryllium piston thinner than a human hair into a 5 millimeter-long tube filled with xenon gas, producing a shock with characteristics similar to those that emerge from supernovae. The researchers use the experiments to test computer models of the shocks.

SHOCK PREDICTION

Working with A&M's Ryan McClarren and Carolyn Kuranz, as well as Michael Grosskopf, Erica Rutter and Ben Torralva at Michigan, Stripling once again fit a BMARS surrogate model to outputs generated by HYADES, a physics code that contributes to the CRASH computer model. But instead of completely accepting or rejecting each input point, as BMARS did with CAM, the HYADES emulator assigns each point a weight. The weight takes into account all the uncertainty in the problem, including in the emulator itself, Stripling says. The result is a weight assigned to each of the uncertain inputs the algorithm sampled, with each weight proportional to the likelihood the simulation will replicate experimental results if it's run at that sample.

To verify the calibration procedure, the researchers ran the BMARS emulator to predict shock breakout – the time, measured in trillionths of a second, it takes laser energy to pass through the beryllium disc and send a shock out the opposite side. They compared the emulator's prediction with shock breakout data from eight actual CRASH experiments in what researchers call "leave one out" tests: in eight runs, the emulator calibrated the unknown inputs on data from seven CRASH shots to predict the eighth, omitting a different one each time. If each of the eight predictions is accurate, then the model should more accurately calculate uncertainty when predicting a ninth, as yet untried, shot.

"The problem was highly clouded with uncertainties, but this procedure knocked that down quite a bit," Stripling says – by as much as 27 percent, by one measurement.

To test the emulator's ability to predict new, untried experiments, the researchers also produced shock breakout time estimates with varying values for beryllium disc thickness and laser energy. The results were consistent with real-world data trends.

The Livermore practicum – and one at Argonne National Laboratory in 2011 with applied mathematician and UQ researcher Mihai Anitescu – have recast Stripling's position at A&M. "I'm taking the role as the applied mathematician or uncertainty quantification guy on projects," he adds.

Adams, Stripling's doctoral advisor, says his student excels at using the tools he's collected in his practicums and will help transform them into novel ones. "If you can combine the power of some of these statistical models with your knowledge of the underlying physics of the phenomena … there are significant gains to be made" in improved uncertainty quantification.

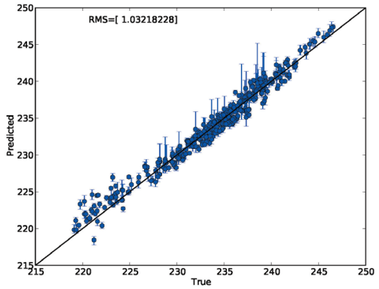
"The sky's the limit for Hayes," says Adams, a professor of nuclear engineering. "He's exceptional."

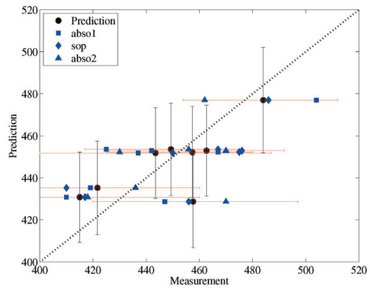
Stripling, Johannesson says, may be part of a new generation of computational scientists who can cross disciplinary lines to incorporate UQ into their engineering codes from the start rather than as an afterthought. Stripling seemed hesitant at first, Johannesson adds, but "he realized how important this is. UQ is getting more and more attention as something that needs to be tackled. I hope he keeps it up."

Johannesson needn't fear. "There's uncertainty quantification going on in every kind of science," Stripling says. "That's why I'm interested in it – because of the rich variety of potential fields I could find myself contributing to one day."

First, Stripling is tackling some other things, like his wedding this spring to Jenny Baker, a fellow Aggie now working in Dallas. And of course, there's his doctoral dissertation. While he knows the focus is UQ, the precise topic is still up in the air.

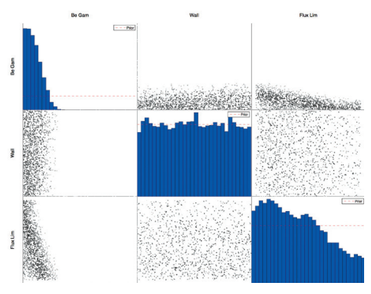
"There are way too many uncertain inputs," Stripling joked. "I need to zero in on something and reduce my dimensionality." Given his instincts, it won't be long before he picks a target.





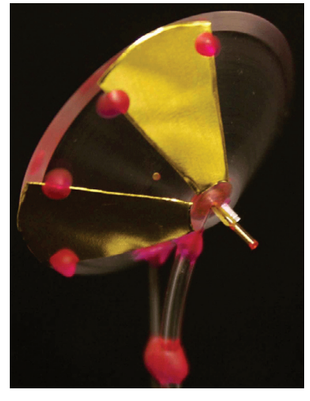
Left: This graph compares BMARS predictions of long-wave radiation calculations to the true value. A perfect BMARS prediction would lie on the 45-degree line. The error bars represent the emulator's uncertainty in predicting each value. Note that the RMS error is less than a tenth of a percent for these data.

Right: This graphic compares a model's prediction of shock location with measurements made in a laboratory. A perfect prediction would lie on the dashed 45-degree line. Horizontal error bars represent uncertainty in the physical measurement and vertical error bars represent predictive uncertainty. Three measurements (abso1, abso2 and sop) per experiment provide some redundancy and reduce predictive uncertainty in the model.



Left: This figure illustrates the posterior distribution of three uncertain inputs to the CRASH laser tube problem. The main diagonal compares each input's posterior distribution (which is informed by measured data) to its prior distribution. The scatter plots show how each variable interacts with the other two variables. The darkness of each sample is proportional to its weight, or the likelihood that it will generate accurate predictions of future experiments.

Right: The University of Michigan's Center for Radiative Shock Hydrodynamics uses powerful laser pulses to drive a beryllium piston thinner than a human hair, at right, into a gas-filled tube, producing a shock similar to those that emerge from supernovae.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ALUMNI PROFILES

ALUMNI SPAN THE GLOBE

Livermore Alumnus Fields Hard Problems and Hockey Pucks

Jeffrey Hittinger
Lawrence Livermore
National Laboratory

In a way, JEFFREY HITTINGER spends his life at two extremes. As a Lawrence Livermore National Laboratory (LLNL) computational scientist he focuses on the physics of plasmas – searing clouds of speedy ions and electrons – for fusion energy.

Off the job, he's often on the ice, tending goal for a San Francisco Bay-area amateur hockey team. Instead of simulating flying particles, he's blocking or catching flying pucks.

His two interests share a fast pace – extraordinarily fast for plasmas – and a challenging nature, Hittinger says. "I'm attracted to difficult things," he adds. He pauses, then laughs. "I'm a goalie, so maybe I'm interested in difficult, high-pressure things."

Likewise, "we get to work on hard problems" at the lab's Center for Advanced Scientific Computing (CASC), Hittinger says. And like pucks flying in from unexpected directions, "there are always new problems coming at you."

Hittinger, a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient from 1996 to 2000, creates and tweaks computer algorithms that emulate and elucidate aspects of some of the world's most complex experiments.

"It's a mixture of my background and what I stumbled into when I came to the lab," Hittinger says. As a graduate student, he used gas kinetics to model fluid mechanics. Lab personnel recruited him to improve fluid plasma models for laser-driven inertial confinement fusion (ICF), the goal of the National Ignition Facility (NIF).

In NIF's stadium-sized building, powerful lasers shoot into a hohlraum, a thimble-sized container holding a BB-sized capsule of frozen hydrogen isotopes. The laser pulse generates powerful X-rays, imploding the pellet with tremendous pressure and heat. The hydrogen atoms fuse, releasing energy in a process similar to that powering the sun.

"For ICF to work, you have to get a nice, clean implosion," Hittinger says. "To do that, you need all the energy you're putting into the system to go where you want it to go." Plasma, however, can interact with the lasers, scattering or reflecting them.

Hittinger has helped improve laser-plasma interaction simulation codes, sometimes replacing or refining the hydrodynamic algorithms at their heart. He's worked on adaptive mesh refinement (AMR) to focus computation on the most interesting areas, like where instabilities occur.

VALHALLA, one of Hittinger's latest ICF projects, combines AMR with an efficient algorithm for solving the Vlasov-Poisson equations, which describe the self-consistent evolution of plasma particle distributions. The goal: cut the computational cost of simulations in phase space – up to three spatial and three velocity dimensions – to make such simulations practical. "We haven't demonstrated yet that it's absolutely going to give you a speedup" in computation, Hittinger says, but work is continuing.

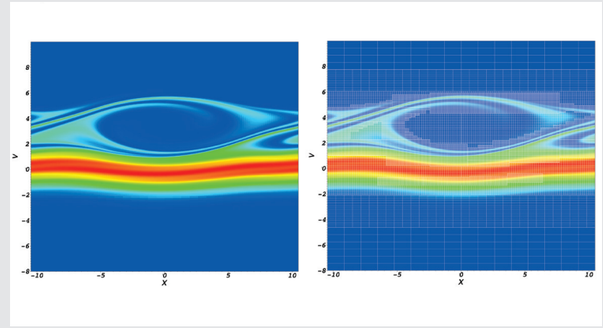
Hittinger's ICF work led him to magnetic confinement fusion, which trades a tiny pellet for a giant plasma cloud, hotter than the sun, swirling through a donut-shaped chamber called a tokamak. In the core, a magnetic field confines the plasma while radio waves heat it enough to strip away electrons and fuse hydrogen nuclei.

Hittinger works on kinetic models for the plasma edge – where the magnetic field doesn't confine the plasma – which varies significantly. To be most efficient, the models' computational grids should follow the magnetic field lines, Hittinger says. "Of course, the magnetic field is not a simple structure, especially in a tokamak and certainly not in an edge geometry."

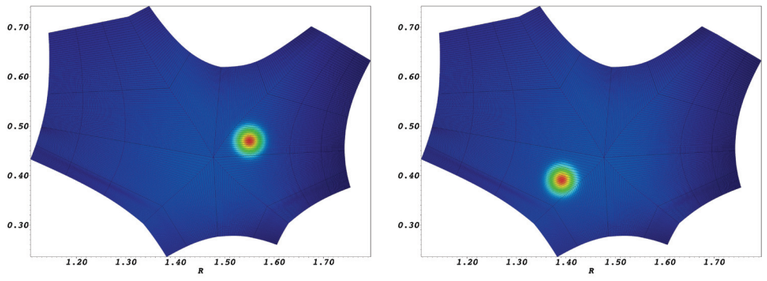
Nonetheless, COGENT, the code Hittinger is developing with researchers from LLNL and Lawrence Berkeley National Laboratory – including fellow DOE CSGF alumnus Daniel Martin – already has shown good agreement with some theoretical benchmarks. It uses high-order methods on mapped grids to solve the gyrokinetic Vlasov-Poisson equations, a plasma model suitable for an imposed magnetic field.

VALHALLA and COGENT are just two of the many "pucks" that have Hittinger's attention. He's also helped plan for the Fusion Simulation Program, a proposed multiyear, multi-institutional effort to develop a predictive, whole-device tokamak model. The project would couple codes portraying different physical properties, much as climate researchers join components into community models.

It's a full plate for someone who didn't picture himself at a national laboratory when he started graduate school. "If it weren't for the CSGF, I probably wouldn't have come to the lab," Hittinger says. "I'm glad I did, because it fits my personality and my skill set. We do interdisciplinary things, and they're hard problems. I don't think there are many opportunities for that."



These visualizations show Vlasov-Poisson simulation results for a bump-on-tail instability problem, where a non-equilibrium distribution of electrons drives an electrostatic wave. The left image shows particle density as a function of space and velocity. The right image shows the adaptive mesh refinement computational grid that calculates conditions with greater resolution around the resonant particle trapping region and with less resolution elsewhere, conserving computer resources.



These visualizations show successful, high-order propagation of an isolated disturbance through the "X-point" – a singular point in the tokamak magnetic field geometry where the flux surface that separates regions of closed and open field lines (the separatrix) intersects itself. This is an important test for the high-order, mapped-multiblock finite volume algorithms developed for gyrokinetic edge simulation.

Richard Katz
University of Oxford

Delving into the Deep Earth

RICHARD KATZ may spend his time contemplating what happens far below Earth's surface now, but his choice of research area wasn't a particularly deep decision at the time.

"There was never a moment when I said, 'This is what I'm interested in studying – geophysics of the deep Earth,'" says Katz, a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient from 2001 to 2005. "It was an evolution over probably my whole life. Small decisions led me to where I am."

Here's where Katz is: a lecturer in the Department of Earth Science at England's University of Oxford. He uses computers to model processes occurring deep in the Earth, like plate tectonics, mantle convection and the phase changes that drive magma creation and movement. The models are used to make measurable predictions. The challenge for deep-Earth researchers, Katz says, "is to connect the processes that are happening in places beyond our ability to observe with the consequences of those processes, which are accessible" to measurement and quantification. A volcano, for example, is an observable manifestation of processes happening far below ground.

In a recent project, Katz and his colleagues studied how the heterogeneous nature of Earth's mantle – the rocky layer between the crust and the molten core – affects magma genesis and migration. As crustal rocks are pushed deep below the surface into the convecting mantle "it's like a taffy pull," Katz says. "You have stripes and blobs of different composition and those different compositions have different melting properties," complicating magma's movement below the surface.

In a paper published online in the journal *Earth and Planetary Science Letters*, Katz and doctoral student Samuel Weatherley modeled magma-mantle dynamics and melting reactions beneath mid-ocean ridges. The model says that when mantle heterogeneities melt preferentially, the magma creates isolated channels that provide a path for rapid ascension toward the surface. That flow may be how magma moves, in isolation from the surrounding mantle, to the boundary between the crust and the mantle along the mid-ocean ridges. The model also suggests that pools of magma get trapped at the boundary of Earth's solid outer layers. The pools feed volcanoes or solidify, making the mantle more heterogeneous.

Katz and his research group use similar techniques to model structures near the other temperature extreme: ice sheets and glaciers. Ice and subsurface materials share many of the same physics, including flows and phase changes under pressure. While scientists recognize the role ice shelves have in Earth's climate, there's much they don't know about them.

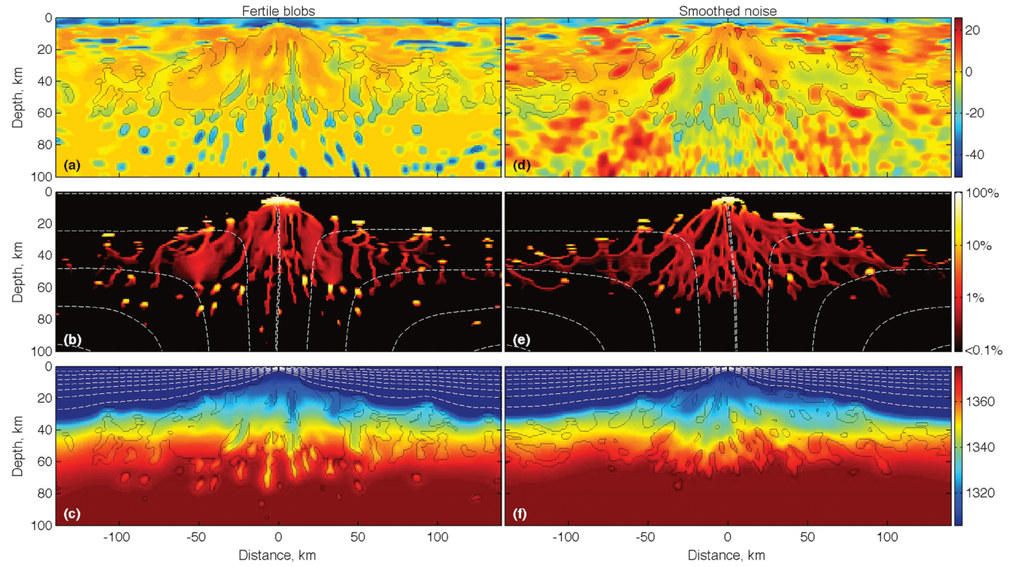
In another climate-related project, Katz's group is developing computational models of how "volatiles" – water, carbon dioxide and other substances – transfer from the solid Earth to the oceans and atmosphere. "In the long term, over millions of years, climate is really controlled by the solid Earth," Katz adds. "The atmosphere is the tail and the solid Earth is the dog."

Katz develops his calculations with PETSc (Portable, Extensible Toolkit for Scientific Computation), a software library for large-scale simulations. He first learned to use this toolkit – and other science software – through the DOE CSGF, especially during his 2003 practicum at PETSc's birthplace, DOE's Argonne National Laboratory. "I'm interested in spending my time learning about the Earth, so the fact I can leverage these sophisticated tools by world leaders in computation means I can solve problems without having to create all the machinery myself," Katz says. "The practicum was a key step in my thesis and subsequent work."

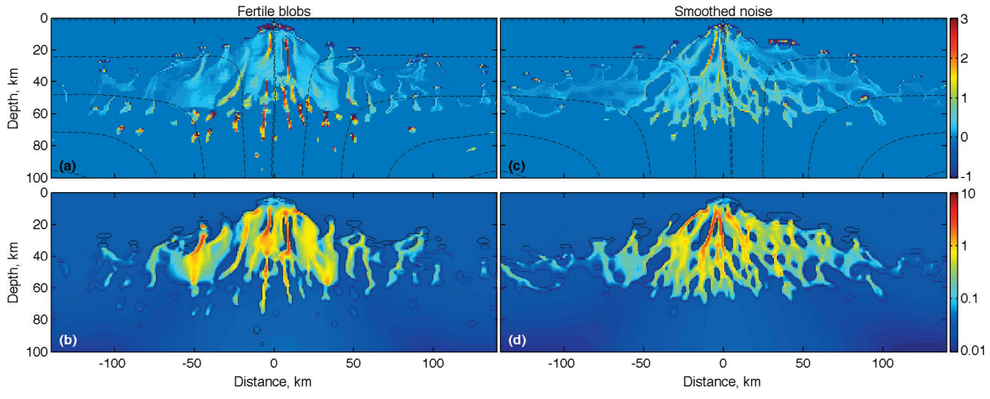
Another key step was Katz's National Science Foundation postdoctoral research fellowship at Oxford's rival, the University of Cambridge. The experience helped lead to his faculty appointment.

Katz calls his research group FoaLab to honor his grandfather, Piero Foa, an endocrinologist who fled fascist Italy for the United States, where he made key discoveries about Type I diabetes. Foa stoked his grandson's curiosity, sharing everything from dissecting frogs to building sand volcanoes. Foa was 94 when he died in 2005, shortly before Katz received his doctorate.

"I think he would be happy to see me working in a field that's at the cutting edge," Katz adds. The use of large-scale computing to study problems in nature is "one of the ways science is advancing most rapidly."



Representative output from two ridge simulations. Panels (a) and (d) show the compositional perturbation of solidus temperature as a physical proxy for chemical heterogeneity. The boundary between partially molten and unmolten mantle is marked in black. Panels (b) and (e) show the porosity field with a log-scale color bar; porosities below 0.1 percent are shown as black. Mantle streamlines are overlain in white. Panels (c) and (f) show the mantle potential temperature, with a color scale chosen to highlight temperature variability in the asthenosphere – the upper layer of the mantle. Temperature contours within the lithosphere (the layer above the asthenosphere) are overlain in white. The grid spacing is 1 km in both simulations.



These images show melting rate and magmatic flow speed for two ridge simulations. The simulation on the far left was begun with a random array of fertile blobs while the simulation on the near left was begun with a smoothed, random-noise field. Panels (a) and (c) show the melting rate in units of 10^{-3} kg/m^3/year. Panels (b) and (d) show the magnitude of magma velocity in units of meters per year. Note that the color scale is logarithmic in the velocity.

Jimena Davis
U.S. Environmental Protection Agency

Tackling Uncertainty in Chemical Vulnerability

If there's a theme to JIMENA DAVIS' postdoctoral research for the U.S. Environmental Protection Agency, it may be exposure.

Davis researches ways to calculate uncertainty in computer predictions of how chemical exposure affects human health. She's also learning about life in a government research enterprise.

"It has exposed me to different ways of thinking about things," says Davis, a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient from 2004 to 2008. "It's exposed me to a lot of different types of science that I didn't experience during grad school."

As a Cross ORD (Office of Research and Development) postdoctoral fellow, Davis works with scientists at both the National Center for Computational Toxicology (NCCT) and the National Exposure Research Laboratory (NERL) in Research Triangle Park, N.C. "They're working on the same project, but a lot of the time they work in their own offices and come together toward the end to combine results," Davis says. "With the Cross ORD program there's more collaboration the entire time" – with Davis providing the connection.

It can be tricky turf to navigate. Davis' NCCT mentor, Woodrow Setzer, is a statistician, while her NERL mentor, Rogelio Tornero-Velez, chiefly develops models. "One may think, 'well, we don't really need to do a full statistical analysis.' The other side might say, 'no, we need to go through X, Y and Z.' I'm in the middle trying to find common ground."

For Davis, the collaborative approach is good training for taking simulations all the way from development to analysis. For the EPA, it's a shorter path to computer calculations that supplement and focus expensive lab research and guide officials' regulatory rulings.

Davis' research puts a number on how much a model can be trusted. The physiologically based pharmacokinetic (PBPK) models she works on predict the way human bodies absorb, distribute, metabolize and excrete chemicals. They're the middle component in "linked exposure-to-effects" models. The first parts, exposure models, use data from animal experiments or human activity to estimate how much of a chemical the body takes in. Those results feed into the PBPK model, which calculates how much of the chemical settles in body tissues. Finally, PBPK output goes into an effects model, which estimates adverse consequences.

Davis and her colleagues test their methods by studying pyrethroids, a common class of insecticides. They're extrapolating data from rat experiments to humans and inputting the results to the linked models.

That extrapolation, however, is one way uncertainty can be introduced into the results. It also can arise from poorly measured or unknown inputs to the models and from imprecise calculations. Another uncertain factor is variability – the fact that each human body will respond somewhat differently to chemical exposures.

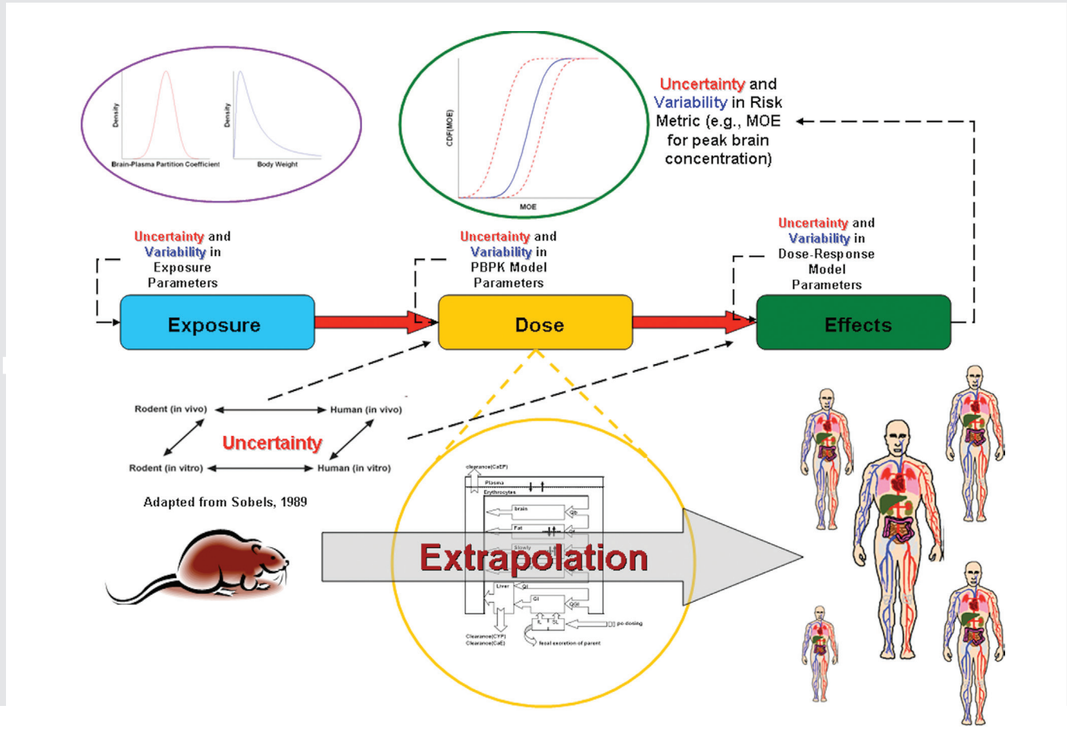
To cope with variability and uncertainty, Davis and her fellow researchers develop mathematical and statistical methods to intelligently sample the many combinations of parameters and characteristics. "We have uncertainty distributions and variability distributions," she says. "You can sample the parameters from those distributions, run them through the model and come up with distributions for your predictions as well." Because of uncertainty, models can't produce a single answer to questions like what level of exposure is safe for a chemical. They can provide only a range of possibilities.

That doesn't always satisfy officials who base decisions on the results. "They might want just a single value," Davis adds. "When you say, 'Well, no, it's more in this range,' that sometimes doesn't go over as well." Nonetheless, in the end "you do want to come up with something that can be used in policy."

Davis chose her post partly because it keeps her close to North Carolina State University, where she earned her doctorate, and to her home state of South Carolina, where she still has family – and people seeking math advice. In her hometown, "everybody kind of knows everybody, so I get calls and emails from a lot of kids," Davis says. "I might know their parents or their parents know my parents, and they're like, 'Oh, yeah, Jimena can help out.'"

Davis is glad to. "I definitely want to figure out even more ways or opportunities to mentor young women, especially, but young people in general and motivate them to consider careers" in science, technology, engineering or math.

Again, it's all about exposure.



Uncertainty can be introduced along multiple points in a linked model of how chemical exposure can affect human health. Exposure models calculate how much of a chemical the body absorbs. A physiologically based pharmacokinetic (PBPK) model predicts how chemicals are absorbed, distributed, metabolized and excreted. An effects model calculates adverse outcomes. In some cases, computer models help extrapolate data from rodent tests to consequences for humans.

WINNING ESSAYS

ENCOURAGING COMMUNICATION THROUGH AN ANNUAL WRITING CONTEST

WINNER

A PLACE IN THE SUN

by Kenley Pelzer

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.

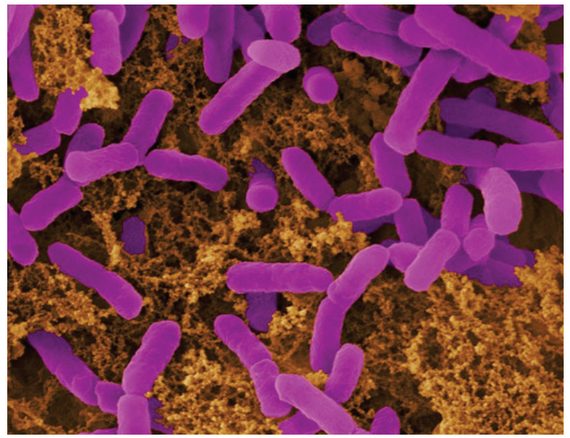
In addition to recognition and a cash prize, the winners receive the opportunity to work with a professional science writer to critique and copy-edit their essays. The latest winning essays are published here.

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

MY SON WAS BORN in the winter in Chicago. Our neighborhood was a wasteland of gray skies and leafless trees, and it was much too cold outdoors for a newborn. Confined to our small apartment, I sang to my baby about flowers and trees and sunshine. As he gazed at the plastic sun attached to his activity mat, I counted the days until spring.

When warmer weather finally came, we made our first trip to the neighborhood park, and I was not disappointed. He was enthralled by his discoveries: the rough bark of trees, the leaves that rustled around us, and the moist dirt that soon covered his hands and clothes. His favorite toy was the grass. Ignoring the swing set, he sat for 20 minutes in a patch of grass, pawing at the ground with his tiny and uncoordinated hands. I plucked out a few blades of grass for him, and he stared with pure rapture, marveling at the miracle in front of him. As I watched, I was struck by the fact he wasn't alone in his amazement. The chemical processes occurring within each blade of grass have captured the wonder and curiosity of thousands of scientists.

Photosynthesis converts the energy of the sun into the chemical energy each blade of grass – in fact, in every plant on earth – needs to survive. The Earth's plants, algae, and bacteria capture approximately 100 terawatts of energy each year – about six times the power the world's people consume each year as we pour energy into electrical needs, transportation and more. As the dangers of fossil fuel consumption become increasingly clear, armies of scientists are struggling to find safe and cost-effective ways to meet human energy needs. In their quest for alternative energy sources, they look enviously at the ability of photosynthetic organisms to capture the energy of the sun.



Chlorobium tepidum bacteria, magnified 2,600 times with a scanning electron microscope, are known for their ability to transfer solar energy with nearly 100 percent efficiency.

Although photosynthesis has been heavily researched, it's still a mystery why it's so efficient. We know that plants are effective at converting solar energy to a form of energy they can use. But how? And if we understand how, can we learn to efficiently capture solar energy ourselves?

These questions aren't easy to answer. Ideally, we'd like to know how a plant processes a single photon (a tiny fragment of light). Understanding photon processing will provide insight into how sunlight provides useful energy to a plant – or to a solar-powered car or home heating system. Unfortunately, the size of photons and the complex laws governing their behavior make it extremely difficult to design experiments that study a single one.

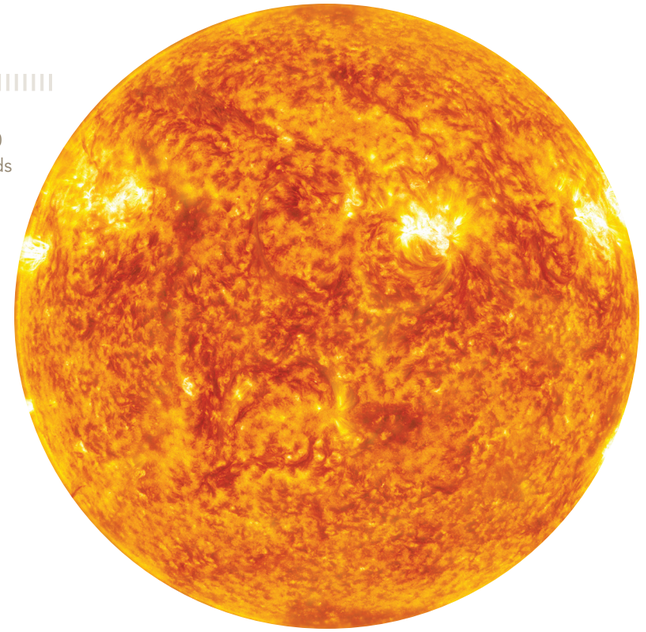
Fortunately, there is another way.

Rather than using experiments to study photons, we can describe much of what we understand about light with systems of mathematical equations. These equations are often impossible to solve with pen and paper, but with modern computers we can depict sunlight's effects mathematically. These computational calculations can help explain why plants are masters at turning sunlight into useful energy.

To attack the problem, we first write a computer program with equations describing solar energy processing. These programs are not necessarily long or complicated; a few well-chosen equations can model energy transfer. Then we make adjustments to account for the environment inside a particular photosynthetic organism. When the program is ready, just a page or two of computer code contains a lot of information about how sunlight is converted into a form of energy that the organism can use. Then the computer does all the hard work: solving equations and simulating the behavior of a multitude of molecules.

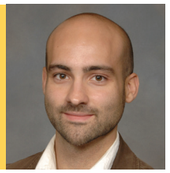
The results could have real impact. Recently, researchers have focused on bacteria that live in low-light environments and transfer solar energy with nearly 100 percent efficiency. Since the best solar cells operate at a mere 20 percent efficiency, scientists clearly stand to learn a great deal from these extraordinarily resourceful organisms. With hard work – and a lot of computers – the calculations examining these bacteria may help humans use solar energy better, decreasing our dependence on fossil fuels.

How bacteria and plants use solar energy efficiently remains mysterious in many ways, and mimicking this process with man-made devices presents a formidable challenge. Yet as the current energy crisis becomes urgent, solar energy research is receiving more and more attention. Research in this area requires top-notch scientific methods to explore how we can harness the power of our sun, and computational calculations are one of the important tools that we can use to face this challenge. By using the power of computers to tackle the mysteries of nature, we may one day understand the miracle that occurs inside each blade of grass – and use this understanding to create a sustainable energy source for our babies' generation and beyond.



The sun contributes approximately 100 terawatts each year to the energy needs of plants, algae and bacteria.

HONORABLE MENTION



A NEW VIEW ON OLD LIGHT

by Paul M. Sutter

TRUE STORY: About 13 billion years ago the entire universe had a temperature of more than a million degrees Celsius and was about the size of a peach.

How can we possibly know this? The answer is as near as your television. Here's why.

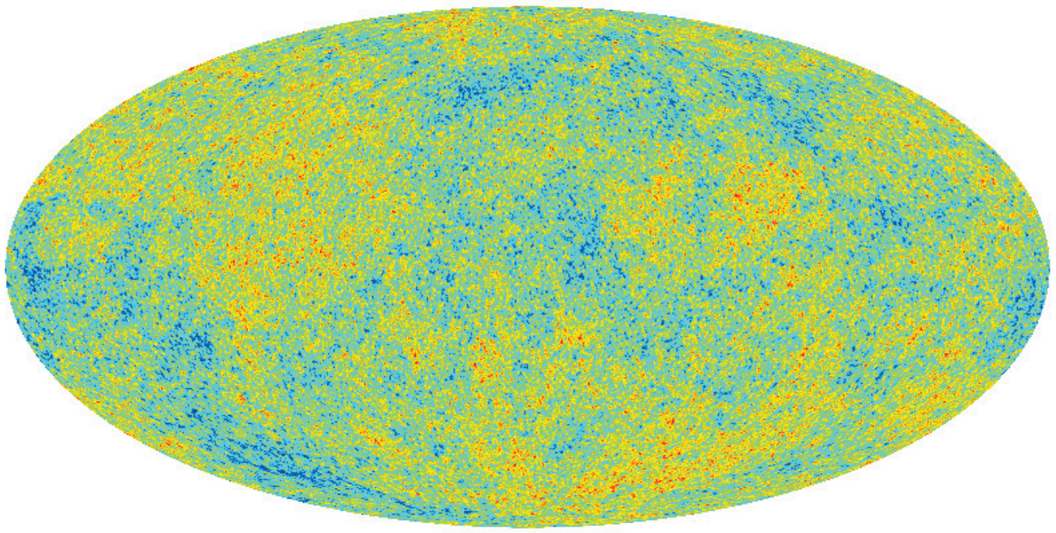
The early universe was so hot and dense that atoms couldn't even form. As soon as a proton captured an electron – forming hydrogen – extremely high-energy radiation ripped it off again. Thus, the universe was a plasma, the same state of matter as found in the surface of the sun or in a lightning bolt.

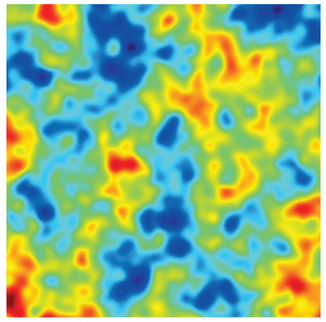
The universe remained as a plasma for about 300,000 years. Eventually, it cooled and expanded enough that the first stable atoms could form and high-energy radiation could roam without constantly knocking into them.

This radiation started life as ultra-short-wavelength gamma rays, but as the universe grew old and stretched out, the radiation stretched out too, shifting down the energy spectrum to X-rays, through the ultraviolets, blues, reds and infrareds all the way down to microwaves. As this freed radiation traveled the universe, clumps of matter coalesced to form galaxies, stars, planets, you and me.

Some radiation didn't survive long. Gas in a newly formed galaxy absorbed it or a black hole pulled it in, to be lost forever. But most remained, and after a journey of 13 billion years, some of that radiation finally comes to rest ... in our TV antennas.

That's right: About 20 percent of the static you see on an old TV is radiation from this so-called Cosmic Microwave Background (CMB). In fact, this leftover radiation from the Big Bang is by far the brightest thing in the universe. If our eyes could see microwaves, it would outshine the stars, the sun, and anything made by humans. That's how we know the primeval universe was peach-sized and hot: It's the only explanation for the way this radiation appears today. Studying the CMB helps us understand the universe's earliest moments.





A view of the Cosmic Microwave Background as the Planck satellite sees it and an enlarged portion of the image. Small differences in temperature reveal the structure of the very early universe.

Scientists have observed the Cosmic Microwave Background for about 50 years. The latest effort, from the European Space Agency, is based on the Planck satellite, which tirelessly sweeps across the heavens, measuring and probing this old, tired light.

The satellite, launched in May 2009, is good – too good, in fact. It's performing beyond expectations, constantly delivering an enormous amount of data even past its expected lifetime. We must squeeze every last bit of insight out of these data if we are to understand our early universe. That requires new algorithms – mathematical recipes – and computational techniques to handle, categorize, filter and process this information into meaningful science.

One essential algorithm I helped develop is the spherical convolution, named because Planck sees the sky as a complete sphere. In effect, this algorithm "smoothens" the microwave signal, which is important for removing noise and holes in the data and for identifying important features of different sizes.

I invented a new type of spherical convolution algorithm – one that runs on Graphics Processing Units (GPUs), the same hardware that makes modern video games so stunning. That means our algorithm is not only fast – about 20 times faster than older approaches – but also cheap; a new GPU costs only about $500, peanuts for a multi-million-dollar research program.

Our new algorithm has many applications besides studying the young universe. Need to use a satellite to search the Earth's surface for oil or mineral deposits? We can speed you up. Trying to make artificial eyes correctly compute reflections off round surfaces? We can help. Trying to use the latest in medical imaging to diagnose cancer? Yup, that too. All these applications rely on spherical convolutions, and the faster the better.

This is just one example of the serendipitous effects of these primary science missions. We're constantly pushing the boundaries of hardware and software to acquire and understand our data. New machines, new techniques, new tools and new algorithms all come along at no extra charge when we do our best to look up into the night sky and see as far as we can into the past.

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

HOWES SCHOLARS SALUTED FOR RESEARCH AND SERVICE

2012 WINNERS
CAROLYN PHILLIPS
& MATTHEW REUTER

Two researchers, one in nanomaterials and the other in theoretical and computational chemistry, are the 2012 Frederick A. Howes Scholars in Computational Science.

The award honors recent doctoral graduates of the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) program for outstanding technical achievements, but also recognizes exceptional leadership, integrity and character – qualities that reflect the award's namesake.

The late Fred Howes, manager of DOE's Applied Mathematical Sciences Program, was an advocate for the fellowship and its goals.

Carolyn Phillips and Matthew Reuter are the 16th and 17th Howes scholars. Phillips was a fellow from 2006 to 2010 and in December 2011 successfully defended her doctoral thesis in Applied Physics and Scientific Computing at the University of Michigan. She now holds the Aneesur Rahman Postdoctoral Fellowship at Argonne National Laboratory and has joined Argonne's Computational Institute.

Reuter, a fellow from 2007 to 2011, received his doctorate in chemistry from Northwestern University in 2011. He's now a Eugene P. Wigner Fellow at Oak Ridge National Laboratory.

Phillips' research has focused on nanomaterial self-assembly. She has created new mathematical frameworks and computational tools to characterize known nanoparticle assemblies and propose designs for novel nanostructured materials, the Howes selection committee wrote in its citation. She already has compiled an impressive list of publications, including a paper featured on the August 2009 cover of the *Journal of Chemical Physics*.

Yet Phillips says she was anxious as she started her fellowship, particularly when it came to climbing the steep learning curve in computational science. "I had conversations with other new fellows where we discussed our shared fear of being found out" for losing their way in a forest of jargon at the first few conferences.

The award recognizes the value of a diverse academic background, Phillips says, especially in computational science, an ideal field for researchers to integrate different disciplines and provide new perspectives. "I also like to think that my background as a naval nuclear propulsion research project officer enables me to see research from a pragmatic perspective, with a mindset toward making an impact."

Reuter's doctoral research looked at transport of electrons in molecules adsorbed onto surfaces, a project that involved applying quantum dynamics, non-equilibrium charge transport and quantum control algorithms to real-world applications. He's also pursued independent projects in such areas as the role of dimensionality on material properties, the scaling of real-space density functional theory algorithms, and the application of diffuse-layer boundary methods to nanoscale photonics problems. He is first author on nine papers appearing in *Nano Letters*, the *Journal of Chemical Physics*, *Physical Review Letters* and other publications.

Reuter "has also distinguished himself as a leader with compassion, commitment and integrity," his award citation reads. His dedication to educating and mentoring undergraduate and graduate students earned Northwestern's Edmund W. Gelewitz Award for Excellence in Research and Service and the Donald E. Smith Award for Excellence in Graduate-Level Teaching. The Howes award, Reuter says, "is an affirmation that I made good decisions in graduate school." It sets the bar high, but "it's nice to know others have confidence in my ability to tackle the challenges" in years to come.

Working in the community, Reuter says, was a way to keep research from consuming his life. He was part of a team that taught introductory science lessons to third- and fourth-grade students in Chicago public schools and he coordinated, prepared and served monthly dinners at an Evanston homeless shelter. "I never thought of these actions as showing 'leadership' or 'character,'" Reuter says, but he's pleased others did and that the Howes award recognizes their value.

Phillips, similarly, has demonstrated leadership throughout her graduate career: mentoring and helping graduate and undergraduate students, establishing new collaborations and spearheading the development of new computational tools. She led the establishment of the Physics Graduate Summer Symposium, a weekly summer seminar series at Michigan designed to give graduate students opportunities to share their research and improve their presentation skills. Phillips also helped administer the GPU summer courses at the Virtual School of Computational Science and Engineering, an initiative connecting numerous universities and laboratories. Phillips also won the 2008 DOE CSGF Essay Contest and spoke at the 2011 Annual Meeting of the Minerals, Metals and Materials Society.

The selection committee chose Phillips and Reuter from among DOE CSGF recipients who completed or planned to complete their doctoral requirements in 2011, either after receiving support for the maximum number of years or finishing the fellowship that year. To be considered, alumni must be nominated by department chairs, advisors or fellowship coordinators at their universities.

The two newest Howes Scholars will receive an honorarium and engraved award and at the 2012 DOE CSGF Annual Conference near Washington, D.C., where they also will deliver lectures describing their research.

ABOUT FRED HOWES

In the 11 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. 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

2011	Alejandro Rodriguez
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

2012 fellows directory
CLASS OF 2012

Carl Boettiger
University of California, Davis
Biology – Ecology and Evolution

Advisor: Alan Hastings
Practicum: Lawrence Berkeley National Laboratory
Contact: cboettig@gmail.com

Scott Clark
Cornell University
Applied Mathematics

Advisor: Peter Frazier
Practicums: Los Alamos National Laboratory and Lawrence Berkeley National Laboratory
Contact: sc932@cornell.edu

Curtis Hamman
Stanford University
Flow Physics and Computational Engineering

Advisor: Parviz Moin
Practicum: Sandia National Laboratories – California
Contact: cwhamman@stanford.edu

Armen Kherlopian
Cornell University
Computational and Systems Biology

Advisor: David Christini
Practicum: Princeton Plasma Physics Laboratory
Contact: ark2010@med.cornell.edu

Kathleen King
Cornell University
Operations Research

Advisor: John Muckstadt
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Fellowship Years: 1997-2001
Current Status: Associate Professor, Department of Civil and Environmental Engineering, 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: Associate Professor, Mathematics, U.S. Naval Academy

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

Timothy Germann
Harvard University
Physical Chemistry
Fellowship Years: 1992-1995
Current Status: Staff Member, Applied Physics and Theoretical Divisions, 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: Senior Engineer, 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 Fellow, 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

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: Senior Staff Engineer, 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: Deceased

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

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

Steven Hamilton
Emory University
Computational Mathematics
Fellowship Years: 2007-2011
Current Status: Research and Development Staff, Oak Ridge 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
Exascale, Asynchronous Communication, Multicore, GPUs, Computational Chemistry, Programming Models
Fellowship Years: 2005-2009
Current Status: Assistant Computational Scientist, 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: Technical Staff Member, 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: Research Engineer, 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: Assistant Professor, Georgia Institute of Technology

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: Aerospace Research Engineer, Air Force Research Laboratory, Space Vehicles Directorate

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

Gordon Hogenson
University of Washington
Physical Chemistry
Fellowship Years: 1993-1996
Current Status: Programming 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

Ying Hu
Rice University
Biomedical Engineering
Fellowship Years: 2008-2011
Current Status: Postdoctoral Scholar, California Institute for Technology

William Humphrey
University of Illinois at Urbana-Champaign
Physics
Fellowship Years: 1992-1994
Current Status: Senior Vice President, Enterprise Systems, NumeriX LLC

Jason Hunt
University of Michigan
Aerospace Engineering and Scientific Computing
Fellowship Years: 1999-2003
Current Status: Lead Scientist – Research, 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: Managing Director, Goldman Sachs

Joshua Hykes
North Carolina State University
Nuclear Engineering
Fellowship Years: 2007-2011

Eugene Ingerman
University of California, Berkeley
Applied Mathematics/Numerical Methods
Fellowship Years: 1997-2001
Current Status: Staff Software Engineer, Life Technologies

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

Amber Jackson
University of North Carolina
Applied Mathematics
Fellowship Years: 2004-2008
Current Status: Postdoctoral Researcher, University of North Carolina at Chapel Hill

Anubhav Jain
Massachusetts Institute of Technology
Materials Science and Engineering
Fellowship Years: 2008-2011
Current Status: Alvarez Postdoctoral Fellow, Lawrence Berkley National Laboratory

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, New York University

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

Benjamin Keen
University of Michigan
Conservation Laws in Complex Geometries
Fellowship Years: 2000-2004
Current Status: Research Staff Member, 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: Subcontractor, Honeywell

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

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

Bonnie Kirkpatrick
University of California, Berkeley
Computer Science
Fellowship Years: 2004-2008
Current Status: Postdoctoral Fellow, Computer Science Department, University of British Columbia

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

Justin Koo
University of Michigan
Electric Propulsion Modeling and Simulation
Fellowship Years: 2000-2004
Current Status: Program Manager, Electric Propulsion Modeling and Simulation, 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, Turville Bay MRI & Radiation Oncology Center

Yury Krongauz
Northwestern University
Theoretical and Applied Mechanics
Fellowship Years: 1993-1996
Current Status: Financial Modeling, 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: Principal R&D Engineer/ Program Manager, 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
Transportation Systems
Fellowship Years: 2006-2010
Current Status: Graduate Research Assistant, Cornell University

Jeremy Lewi
Georgia Institute of Technology
Neuroengineering
Fellowship Years: 2005-2009
Current Status: Software Engineer, YouTube

Benjamin Lewis
Massachusetts Institute of Technology
Computational Biology
Fellowship Years: 2002-2006
Current Status: Graduate Student, Massachusetts Institute of Technology

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

Milo Lin
California Institute of Technology
Physics
Fellowship Years: 2007-2011
Current Status: Graduate Student, California Institute of Technology

Alex Lindblad
University of Washington
Computational Solid Mechanics
Fellowship Years: 2002-2006
Current Status: Engineer, Short Form

Tasha Lopez
University of California, Los Angeles
Chemical Engineering
Fellowship Years: 2000-2001
Current Status: Territory Sales Representative, IBM

Paul Loriaux
University of California, San Diego
Computational Biology
Fellowship Years: 2007-2011
Current Status: Graduate Student Researcher, University of California, San Diego

Christie Lundy
Missouri University of Science and Technology
Physics
Fellowship Years: 1991-1994
Current Status: Research Coordinator, 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
Current Status: Postdoctoral Research Scientist, Center for Neural Science, New York University

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

James Martin
University of Texas
Computational and Applied Mathematics
Fellowship Years: 2007-2011
Current Status: Graduate Student, University of Texas

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

Matthew McGrath
University of Minnesota
Computational Biophysics
Fellowship Years: 2004-2007
Current Status: Postdoctoral Researcher, Department of Biophysics, Kyoto University (Japan)

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: Computational Scientist, Lawrence Livermore National Laboratory

Lisa Mesaros
University of Michigan
Aerospace Engineering and Scientific Computing
Fellowship Years: 1991-1995
Current Status: Director, Automotive Programs

Richard Mills
College of William and Mary
Scientific Computing
Fellowship Years: 2001-2004
Current Status: Research 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: Technical Staff Member, 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: Graduate Student, University of California, San Francisco

Heather Netzloff
Iowa State University
Quantum/Theoretical/Computational Chemistry
Fellowship Years: 2000-2004
Current Status: The Art Institute of Phoenix

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 Simulations (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 Finance
Fellowship Years: 2006-2009
Current Status: Algorithmic Trading, Hudson River Trading

Joyce Noah-Vanhoucke
Stanford University
Healthcare Modeling
Fellowship Years: 2001-2003
Current Status: Lead, Cancer Modeling, Archimedes

Peter Norgaard
Princeton University
Computational Applied Physics
Fellowship Years: 2005-2009
Current Status: Researcher, Agilent Technologies

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

Matthew Norman
North Carolina State University
Climate Computational Science
Fellowship Years: 2008-2011
Current Status: Climate Computational Scientist, Center for Computational Sciences, Oak Ridge National Laboratory

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

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

Geoffrey Oxberry
Massachusetts Institute of Technology
Chemical Kinetics/Transport Phenomena
Fellowship Years: 2007-2011
Current Status: Research Assistant, Massachusetts Institute of Technology

Steven Parker
University of Utah
Computational Science
Fellowship Years: 1994-1997
Current Status: Director, HPC and Computational Graphics, NVIDIA

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
Current Status: Visitor in Chemistry, California Institute of Technology

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: Scientist III, 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

Alex Perkins
University of California, Davis
Mosquito-Borne Disease Dynamics
Fellowship Years: 2007-2011
Current Status: Postdoctoral Fellow, Research and Policy for Infectious Disease Dynamics Program, National Institutes of Health

Carolyn Phillips
University of Michigan
Applied Physics
Fellowship Years: 2006-2010
Current Status: Rahman Postdoctoral Fellow, Argonne National Laboratory

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

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: Graduate Student, University of California, Los Angeles

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

Matthew Reuter
Northwestern University
Theoretical Chemistry
Fellowship Years: 2007-2011
Current Status: Eugene P. Wigner Fellow, Oak Ridge National Laboratory

Clifton Richardson
Cornell University
Physics
Fellowship Years: 1991-1995

Sarah Richardson
Johns Hopkins University School of Medicine
Human Genetics and Molecular Biology
Fellowship Years: 2007-2011
Current Status: Distinguished Postdoctoral Fellow, DOE Joint Genome Institute

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

John Rittner
Northwestern University
Grain Boundary Segregation
Fellowship Years: 1991-1995
Current Status: Manager, 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: Joint Postdoctoral Fellow, Harvard University/Massachusetts Institute of Technology

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: Research Associate, The Scripps Research Institute

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

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

Danilo Scepanovic
Harvard/Massachusetts Institute of Technology
Signal Processing/Cardiovascular Modeling
Fellowship Years: 2007-2011
Current Status: Algorithm Developer, Hudson River Trading

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

Samuel Schofield
University of Arizona
Computational Fluid Dynamics, Hydrodynamic Stability, Interface Methods
Fellowship Years: 2001-2005
Current Status: Technical Staff Member, Lawrence Livermore National Laboratory

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

Robert Sedgewick
University of California, Santa Barbara
Computational Biology
Fellowship Years: 2000-2003
Current Status: Software Engineer, Google Inc.

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

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

Amoolya Singh
University of California, Berkeley
Dynamics and Evolution of Stress Response Networks
Fellowship Years: 2002-2006
Current Status: Scientist II, 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, Box.net

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

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

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

Scott Stanley
University of California, San Diego
Large Scale Data Analysis, Search Engine Technology, Fluid Mechanics, Turbulence Modeling
Fellowship Years: 1994-1998
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
Current Status: Software Engineer, Autodesk Inc.

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

Paul Sutter
University of Illinois at Urbana-Champaign
Cosmology
Fellowship Years: 2007-2011
Current Status: Postdoctoral Fellow, University of Illinois/University of Paris

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

Cameron Talischi
University of Illinois at Urbana-Champaign
Computational Mechanics
Fellowship Years: 2007-2011
Current Status: Graduate Research Assistant, University of Illinois at Urbana-Champaign

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: Radiology Resident, Wake Forest University Baptist Medical Center

Mario Trujillo
University of Illinois at Urbana-Champaign
Two-Phase Flow, Computational Fluid Mechanics and 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: Senior Member of Technical Staff, Sandia National Laboratories – California

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

Stephen Vinay III
Carnegie Mellon University
Application of Smoothed Particle Hydrodynamics to Problems in Fluid Mechanics
Fellowship Years: 1998-2000
Current Status: Manager, T&H Analysis Methods Development, Bettis Atomic Power Laboratory

Joshua Waterfall
Cornell University
Molecular Biology
Fellowship Years: 2002-2006
Current Status: Research Fellow, Genetics Branch, National Cancer Institute, National Institutes of Health

Philip Weeber
University of North Carolina
Interest Rate Derivative Consulting
Fellowship Years: 1994-1996
Current Status: Derivative Consultant, Chatham Financial

Adam Weller
Princeton University
Chemical Engineering
Fellowship Years: 2001-2002

Gregory Whiffen
Cornell University
Deep Space Trajectory and Mission Design, Low-Thrust Mission Design, Nonlinear Optimal Control
Fellowship Years: 1991-1995
Current Status: Senior Engineer, Outer Planets Mission Design Group, NASA Jet Propulsion Laboratory

Collin Wick
University of Minnesota
Computational Chemistry
Fellowship Years: 2000-2003
Current Status: Assistant Professor, Louisiana Tech University

James Wiggs
University of Washington
Physical Chemistry
Fellowship Years: 1991-1994
Current Status: Novum Millennium Organization

Stefan Wild
Cornell University
Operations Research
Fellowship Years: 2005-2008
Current Status: Computational Mathematician, Mathematics and Computer Science Division, Argonne National Laboratory

Jon Wilkening
University of California, Berkeley
Numerical Analysis, Computational Physics, Partial Differential Equations, Scientific Computing
Fellowship Years: 1997-2001
Current Status: Assistant Professor, University of California, Berkeley

Glenn Williams
University of North Carolina
Applied and Computational Mathematics, Computational Biology, Environmental Modeling
Fellowship Years: 1993-1996
Current Status: Assistant Professor, Department of Mathematics and Statistics, Old Dominion University

Eric Williford
Florida State University
Meteorology
Fellowship Years: 1993-1996
Current Status: Weather Predict, Inc.

Michael Wolf
University of Illinois at Urbana-Champaign
Computer Science (High-Performance and Combinatorial Scientific Computing)
Fellowship Years: 2003-2007
Current Status: Technical Staff, MIT Lincoln Laboratory

Matthew Wolinsky
Duke University
Computational Geoscience
Fellowship Years: 2001-2005
Current Status: Clastics Research Team, Shell Bellaire Technology Center

Allan Wollaber
University of Michigan
Nuclear Engineering
Fellowship Years: 2004-2008
Current Status: Staff Scientist, Los Alamos National Laboratory

Brandon Wood
Massachusetts Institute of Technology
Computational Materials Science
Fellowship Years: 2003-2007
Current Status: Postdoctoral Fellow, Lawrence Livermore National Laboratory

Lee Worden
Princeton University
Applied Mathematics
Fellowship Years: 1998-2002
Current Status: Postdoctoral Researcher, McMaster University

Michael Wu
University of California, Berkeley
Social Analytics, Graph and Social Network Analysis, Predictive Modeling, High Dimensional Data Visualization
Fellowship Years: 2002-2006
Current Status: Principal Scientist of Analytics, Lithium Technologies

Pete Wyckoff
Massachusetts Institute of Technology
Parallel Architectures and Distributed Networks
Fellowship Years: 1992-1995
Current Status: Software Engineer, NetApp

Charles Zeeb
Colorado State University
Mechanical Engineering
Fellowship Years: 1993-1997
Current Status: Deceased

John Ziegler
California Institute of Technology
Aeronautics: Reactive, Diffusive, Compressible Flow Supercomputing
Fellowship Years: 2007-2011

Etay Ziv
Columbia University
Computational Biology
Fellowship Years: 2004-2008
Current Status: Medical Student (Resident), Mount Sinai Hospital

Scott Zoldi
Duke University
Analytical Modeling
Fellowship Years: 1996-1998
Current Status: Vice President of Analytic Science, Fair Isaac Corporation

John ZuHone
University of Chicago
Astrophysics
Fellowship Years: 2004-2008
Current Status: NASA Goddard Space Flight Center

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