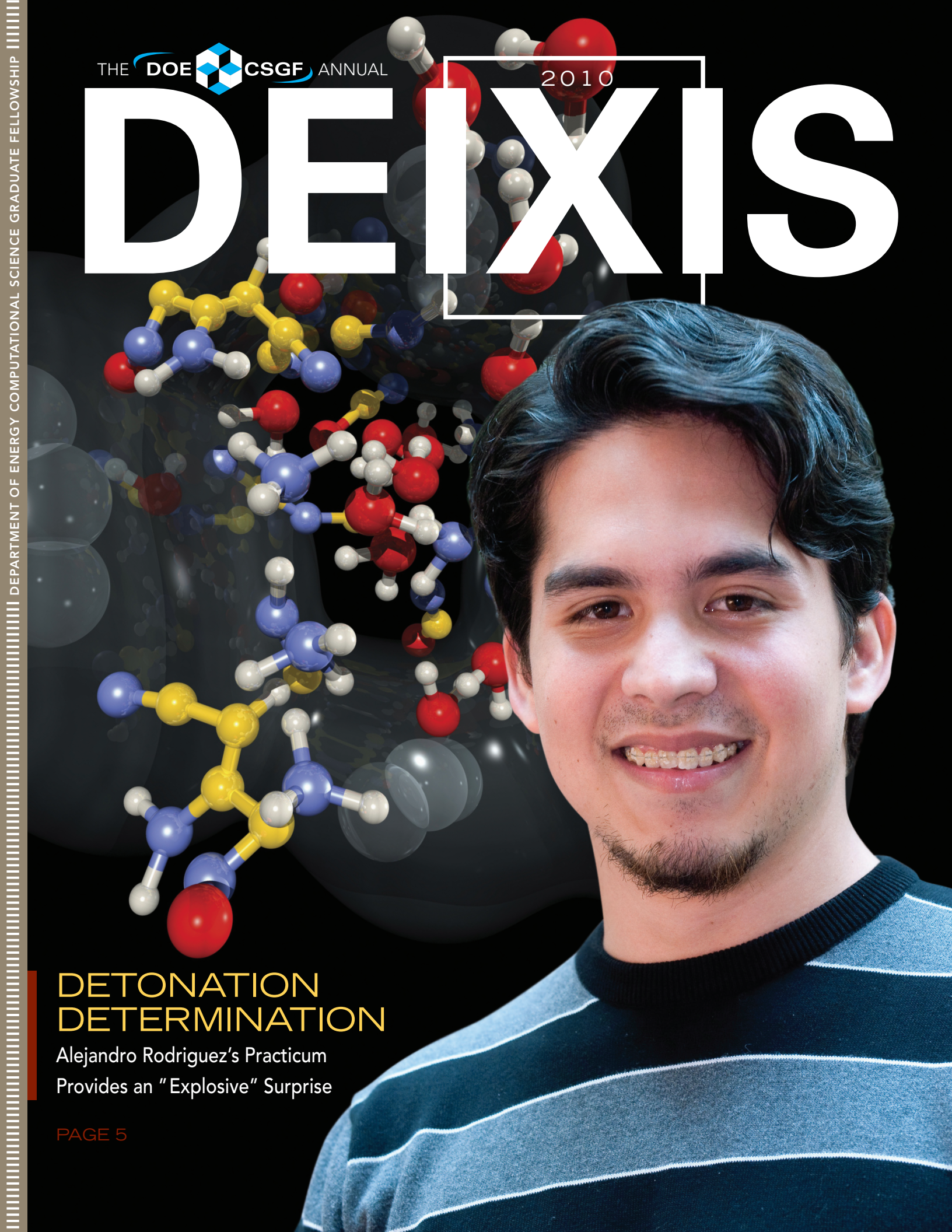
THE DOE CSGF ANNUAL 2010

DEIXIS

DEPARTMENT OF ENERGY COMPUTATIONAL SCIENCE GRADUATE FELLOWSHIP



DETONATION DETERMINATION

Alejandro Rodriguez's Practicum Provides an "Explosive" Surprise

PAGE 5

THE DOE CSGF ANNUAL

DEIXIS

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DEIXIS (ΔΕΙΞΙΣ) transliterated from classical Greek into the Roman alphabet, (pronounced dâksis) 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 (DOE CSGF) program that highlights the DOE CSGF fellows and alumni. The DOE CSGF is funded by the Office of Science and the National Nuclear Security Administration's Office of Defense Programs.

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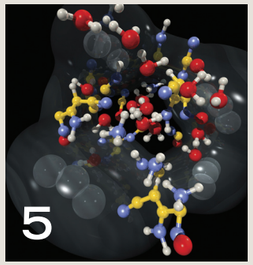

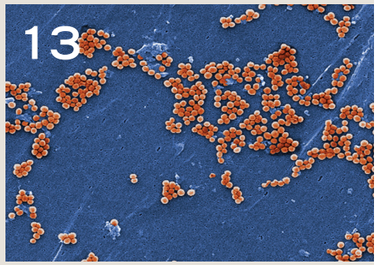

OUR NEW LOOK

Since 2002, *DEIXIS*, the journal of the Department of Energy Computational Science Graduate Fellowship (DOE CSGF), has connected fellows, attracted applicants, and informed academics and policy-makers about computational science and one of the nation's top education programs. Now *DEIXIS* has a new look and a greater focus on fellows and alumni.

The first section features fellows' practicum experiences. The cover story highlights Alejandro Rodriguez, whose practicum produced surprising discoveries about explosive azides. In May, Alex added to his CV with a Proceedings of the National Academies of Sciences paper outlining a novel method to calculate the Casimir force.

Next *DEIXIS* revisits three alumni, including Jon Wilkening, a competitive swimmer whose interest in fluid mechanics is more than academic.

This issue also incorporates winners in an essay competition that encourages fellows and alumni to write for lay readers. This year's top piece, by fellow Anubhav Jain, is of interest to anyone whose laptop battery expired at the wrong time.

Finally, *DEIXIS* reviews 10 years of the Frederick A. Howes Scholar in Computational Science award. Past recipients say the honor set a standard for their careers — a standard 2010 honoree Julianne Chung is sure to exceed.

The redesigned *DEIXIS* is accompanied by the launch of deixismagazine.org, an on-line counterpart where you'll find articles emphasizing computational science at some of the multi-program DOE national laboratories.

We welcome your comments.

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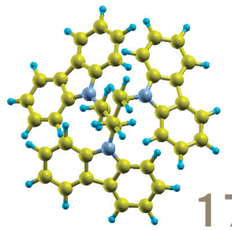
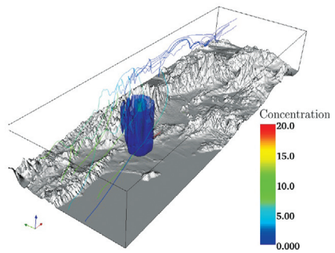
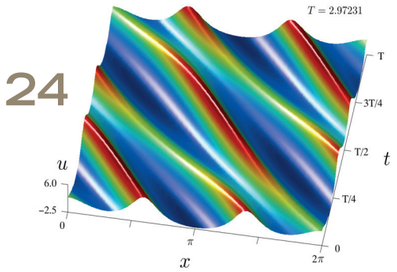
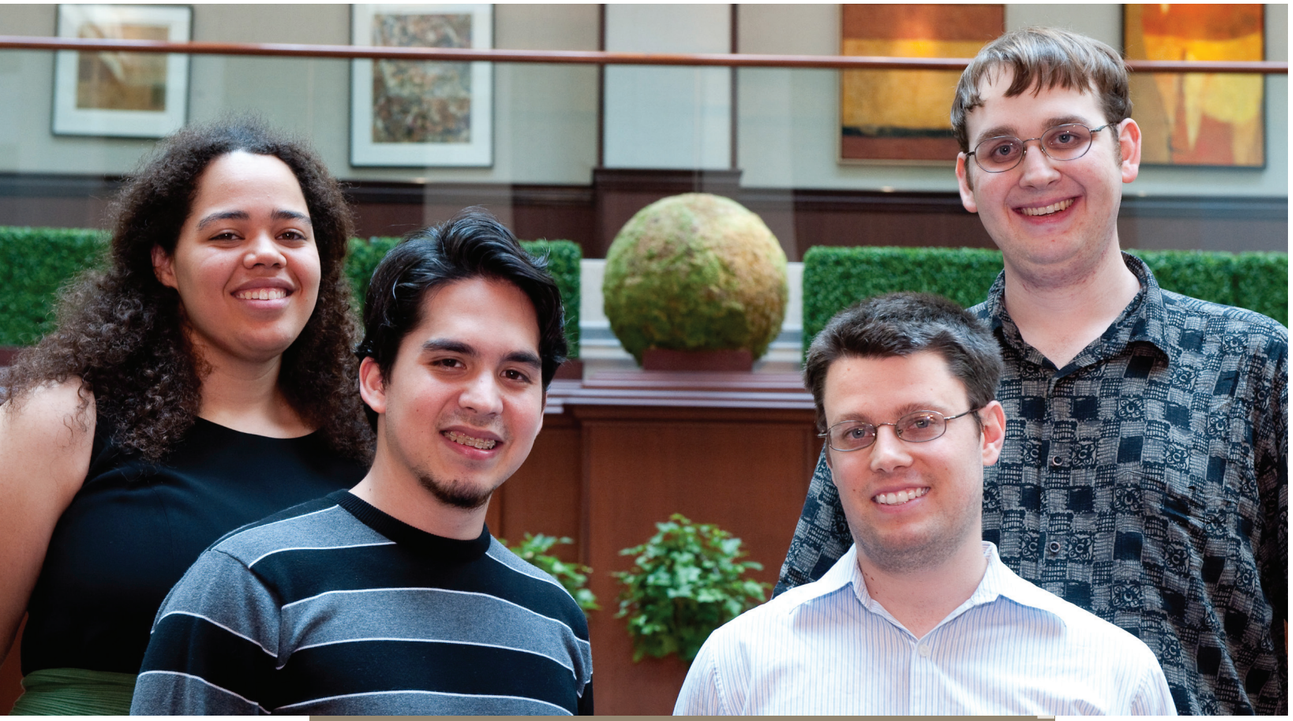






THE PAUSE THAT REFRESHES

THE PRACTICUM IS A VITAL PART OF THE DOE CSGF — A PART THAT HAS BEEN KNOWN TO CHANGE LIVES



Left to right: Sarah Richardson, Alejandro Rodriguez, Jack Deslippe and James Martin in Washington, D.C., at the annual DOE CSGF conference.

THE YOUNG SCIENTISTS in the Department of Energy Computational Science Graduate Fellowship devote years to their doctoral research. For at least three months, however, they break their laser-like focus to try something different.

Fellows travel to DOE national laboratories, usually during the summer, to serve practicums. They work under lab researchers on projects that rarely bear more than a tangential relation to their doctoral studies. The experience lets fellows apply what they know while learning new things; to test their abilities while adding new ones; and to keep one foot in academia while dipping a toe into the world of the national laboratory system.

They return to their universities with new perspectives, new energy and sometimes even new career paths. It's the pause that refreshes and recalibrates.

The Department of Energy Computational Science Graduate Fellowship (DOE CSGF) supports the nation's brightest science and engineering students, allowing them to concentrate on learning and research. The work of more than 200 DOE CSGF alumni has helped the United States remain competitive in a global economy.

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DETONATION DETERMINATION

ALEJANDRO RODRIGUEZ
Massachusetts Institute of Technology
Lawrence Livermore National Laboratory

AS IS OFTEN THE CASE in science, things didn't go quite as planned during Alejandro Rodriguez's practicum at Lawrence Livermore National Laboratory.

But, as it frequently is the case, too, the results were interesting anyway.

Rodriguez is a recipient of a Department of Energy Computational Science Graduate Fellowship and a doctoral candidate in condensed matter theory at the Massachusetts Institute of Technology (MIT). His summer 2008 practicum assignment was to help decipher the electronic structure and atomic-level chemistry when a shock hits cuprate azide. Azides are a class of difficult-to-handle primary explosives often used to ignite more powerful charges in mining and other applications. Lead azide, for instance, is a common part of car airbags.

Defining the structure and chemistry could help researchers understand why heavy-metal azides are so sensitive and release such large amounts of energy.

"Few things are clear about the azides," says Livermore Staff Scientist Evan Reed, who oversaw Rodriguez during the practicum. Experiments are difficult because the materials are dangerous and detonation occurs in mere picoseconds.

"You can't study reactions on that time scale with any existing experimental tools," Reed adds. With the simulations he and Rodriguez worked on, "We're getting the first-ever glimpse at what happens in the process of detonating these materials."

It isn't easy. Such simulations require modeling a cell of dozens of atoms and, more specifically, the degrees of freedom for hundreds of electrons. "You're looking at a very, very, very large system," Rodriguez says. Using density functional theory (DFT), a common electronic structure method, may work, but modeling even a tiny time scale like picoseconds or nanoseconds increases the difficulty dramatically, he adds.

Rodriguez was charged with modeling cuprate azide's inert properties and molecular structure using DFT software coupled with Multiscale Shock Technique (MSST), an *ab initio* multiscale method Reed helped develop. Rodriguez was able to predict the material's ground state energy and other characteristics — and discovered that in detonation it quickly develops metallic properties.
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Rodriguez was able to predict the material's ground state energy and other characteristics — and discovered that in detonation it quickly develops metallic properties.

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"That was a surprise to us and it will be a surprise to many others," Rodriguez says. "That's a good thing. It means we and other people didn't understand the properties as much as we thought we did."

NOT SO EASY AFTER ALL

In short, Reed and Rodriguez believed cuprate azide would be a relatively easy target for analysis, a belief that appears incorrect.

"It was basically metallic at a very early stage — sufficiently early that we couldn't really get very far with the shock simulation," Reed says. As a result, the researchers turned their attention to hydrogen azide, also known as hydrazoic acid, another explosive they believed would be unlikely to have metallic properties, since it consists of only hydrogen and nitrogen.

That assumption also appears wrong, Reed says. Simulations indicate that hydrazoic acid, under detonation, changes from an insulating to a strongly metallic state then back to insulating in a mere 10 picoseconds.

"This is an unexpected result and basically an extension of what Alex did during his time here," Reed says.

Cuprate azide's unexpected behavior kept Rodriguez from achieving his practicum goal of simulating a shock in the material. Even so, "it was a good experience both for Evan Reed and for me. We found the azides we studied became metallic much too early, so studying these systems using the multiscale method would be difficult."

Rodriguez says learning DFT methods complements his usual research into fluctuation-induced interaction in nanophotonic media — how photonic materials respond to light and other electromagnetism. In recent years he's focused on electromagnetic field fluctuations at zero temperature — otherwise known as the Casimir effect or Casimir force.

Dutch physicist Hendrik Casimir predicted the force's existence in 1948. The classic characterization of the force describes two plates in a vacuum, facing each other just micrometers apart. Quantum electromagnetic field fluctuations, Casimir said, should push the two plates together. The effect typically manifests itself only on a tiny scale, but it's become more important with the rise of microelectromechanical systems (MEMS), microscopic machines that often include moving parts.

"Because the Casimir force is usually attractive, these objects can stick together and, therefore, fail," Rodriguez says. Accurate calculations could help develop ways to cancel — or harness — the force. But portraying the Casimir effect mathematically is demanding.

"Five years ago you could count the geometries for which you could calculate the Casimir forces on one hand," says Rodriguez's advisor, Steven Johnson. That's changed since Johnson, fellow MIT professor John Joannopoulos, physics graduate student Alexander McCauley and Rodriguez developed algorithms that for the first time efficiently and accurately compute the Casimir force between objects with complex geometries. Now "If you want to calculate some crazy shape or some complicated periodic structure … we can do it."

Rodriguez "has really been a huge part of this. He really was the one who pushed this work to completion," he adds. Johnson had a crude proof of concept he developed as a postdoctoral researcher, but Rodriguez "was the one who actually turned it into a practical method."

TRACKING THROUGH TIME

Calculating the Casimir force relies heavily, Rodriguez says, on the ability to calculate the Maxwell Green's function, which characterizes electromagnetic response to electronic sources around the surface of an object of interest. One of several methods he, McCauley, Joannopoulos and Johnson developed is based on the finite-difference time-domain (FDTD) scheme. As the name implies, the method calculates equations for electric and magnetic fields as they evolve in time, independent of the frequency of electromagnetic conduction.

The method discretizes the partial differential equations used to calculate the Maxwell Green's function at points around the complex bodies the researchers want to model. The equations are solved in successive time steps as the electric and magnetic fields respond to current pulses at each point. Totaling the electric field results provides the Casimir force, with accuracy depending on computer power and time available to run the problem.

The new algorithms have predicted some surprising Casimir force quirks. In one case the researchers calculated the force between two metal blocks when two parallel plates are placed above and below them. As the plates move closer to the blocks, the Casimir force between the blocks decreases. At a critical point, however, the force begins to increase. When the plates actually contact the blocks, the force is bigger than when the plates were nowhere near.

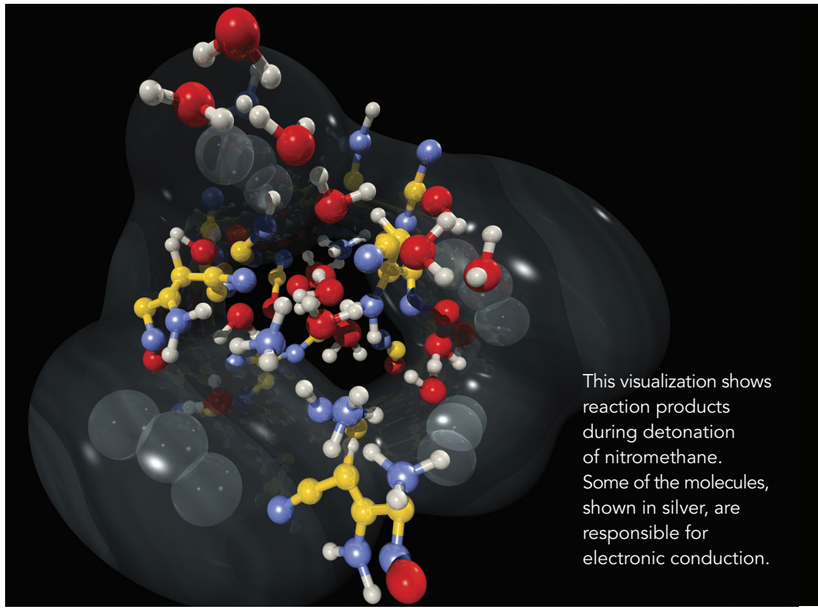
"If you apply the intuition people had before, you would predict completely the opposite results. You would predict the plates would decrease the force between the two blocks," Rodriguez says. Researchers are scrambling to understand the results.

The idea to apply FDTD to Casimir force calculations arose from another concept Rodriguez helped develop: A "Casimir analog computer" capable of calculating the force without supercomputers or tiny plates in vacuum chambers.

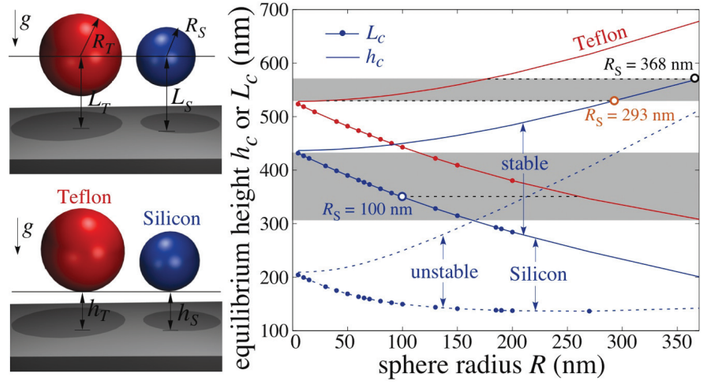
In essence, the computer enlarges the micrometer-sized structures in a standard Casimir force experiment to centimeter scale. Because Maxwell's equations are scale-invariant, there's a mathematical correspondence between calculating the quantum electromagnetics generating the Casimir force in a vacuum and calculating the classical electromagnetic behavior of larger bodies in a conducting fluid.

He and his colleagues propose placing centimeter-scale metal models in a conducting fluid such as saltwater and then bombarding them with microwaves. How the bodies respond should represent how the Casimir force acts on similar bodies at micrometer scale.

The experiment could allow researchers to repeatedly calculate the Casimir force on complex bodies such as capsules and cubes,



This visualization shows reaction products during detonation of nitromethane. Some of the molecules, shown in silver, are responsible for electronic conduction.



Calculations indicate it may be possible to use the interplay between the repulsive Casimir force and gravity to create stable nanostructure configurations levitated above dielectric slabs. This plot shows the stable equilibrium center-surface (L_c) and surface-surface (h_c) separation between either a Teflon (red) or silicon (blue) nanoparticle and a semi-infinite gold slab. It shows that decreasing R acts to increase the surface-surface separation and decrease center-surface separation. The gray areas depict regions in which the L_c or h_c can be made equal by an appropriate choice of radii.
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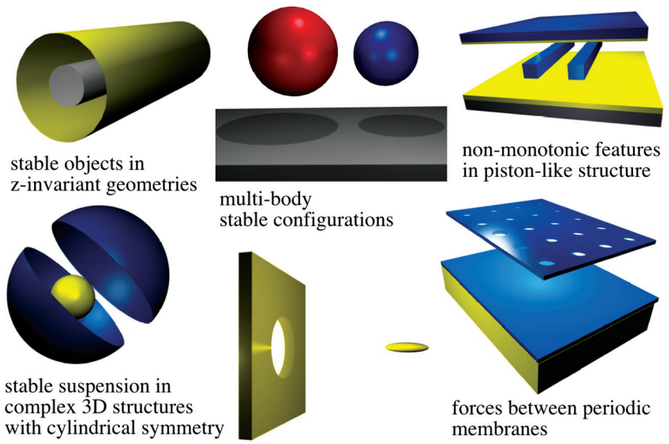
Using mathematical methods he helped develop, Alejandro Rodriguez has calculated Casimir forces in these and other complex structures.



Rodriguez says. "You could probably build many different structures easily and run many, many experiments. The sampling rate is much faster."

Johnson gives Rodriguez and McCauley much of the credit for describing the computer. When the idea came up, "Alejandro got very excited and started talking to everyone. He came back to me a week later and had this whole idea really fleshed out."

Rodriguez's work in Casimir force has created enormous possibilities, Johnson says. "Every time I turn around, Alejandro is calculating another structure or is in another collaboration," he adds. As of early 2010, Rodriguez had contributed to 25 papers — with lead authorship on 11 — in just three years of graduate school. Impressively, four papers appeared in *Physical Review Letters* and for two of those Rodriguez was first author.

Some experimental scientists have expressed interest in building the Casimir analog computer. Rodriguez himself is interested. "I have never in my life had anything to do with experiments, so this is sort of an ambitious goal for me," he says.

ROUNDABOUT ROUTE

It's just the latest ambitious goal in a circuitous life that began in Cuba. Rodriguez's stepfather, a physics professor, was fired for refusing to identify the writers of a letter opposing the Communist government. His mother also lost her teaching job, so the family fled to Mexico with a plan to emigrate to the United States. When the agent hired to get them into the country legally raised his fee, 13-year-old Alejandro and his mother crossed the border illegally and later received political asylum. Fortunately, his stepfather was able to emigrate legally prior to Alejandro and his mother's arrival in the U.S. They settled in the Miami area and became citizens.

Rodriguez says his stepfather's physics background had an indirect influence on his career path. In middle and high schools he was more concerned about fitting in than about grades. The epiphany came his sophomore year, when he took his first physics course.

"I remember coming home to my mom every day and saying, 'Why didn't I study this before?'" Rodriguez adds. He told his school counselor he aimed to be valedictorian, and achieved his goal while taking multiple advanced placement courses. He chose MIT largely because his idol, Richard Feynman, had been an undergraduate there.

Rodriguez expects to graduate in spring 2010 and has accepted a postdoctoral fellowship at Harvard University to begin in June. Besides possibly testing the Casimir analog computer, he's interested in applying numerical techniques the group has developed to interactions in finite-temperature cases, in which one object is warmer than another.

Reed says the practicum gave Rodriguez experience in quantum materials techniques, complementing his doctoral training in quantum electromagnetism. "He may be well-positioned to do some innovative work sort of on the boundaries of those fields," Reed says. "I'm hoping during his postdoc he'll think about how to bridge this gap."

DEALING WITH DIMENSIONALITY

JAMES MARTIN
University of Texas
Sandia National Laboratories – California

FOR JAMES MARTIN, the hard work of observing something in the field or running a laboratory experiment often starts when data are in. His research focuses on finding the conditions that led to the observation or output — and on how trustworthy the findings are.

Martin, a Department of Energy Computational Science Graduate Fellowship recipient, focuses on large-scale statistical inverse problems, which track back to infer what parameters influenced a result.

"That's the classical description for inverse problems," says Martin, a doctoral candidate in computational and applied mathematics at the University of Texas. Inversion is a long-standing — and challenging — mathematical process, he adds. "The thing that's new and interesting is … we're trying to quantify the uncertainty in the inversion."

Uncertainty quantification (UQ) is a hot area in computational science. More powerful computers and improved algorithms have made simulation an important tool for discovery. But if researchers are to rely on simulations, they also must understand the uncertainty inherent in them. UQ puts a number on the degree to which a simulation can be trusted.

"All large-scale, complex models have uncertain parameters that go into them," says Omar Ghattas, Martin's doctoral advisor at Texas. Climate models, for instance, can't precisely calculate the effects of clouds and ice sheets.

"How does one come up with the uncertain parameters in these models?" Ghattas asks. "Typically, it's through the process of an inverse problem: given measurements you try to infer what the parameters should have been."

Martin is applying uncertainty quantification to seismic wave propagation. How these waves reflect off underground strata of earth, rock and fluids helps geologists understand just what's underground, such as oil, gas and mineral deposits.

Making predictions of underground structures from seismic readings is a difficult, classical inverse problem. Martin and Ghattas want to take it a step further by quantifying the uncertainty behind those predictions.

So far Martin is testing his methods on "toy" applications using synthetic seismic data, but he has big plans for his doctoral project. Meanwhile, Martin's research took on an added aspect during his 2008 practicum. For part of the summer he again used seismic data to test his methods.

The problem he confronted was the notorious "curse of dimensionality": As more dimensions are added to a problem — and more parameters that can influence the outcome — the size of the problem grows exponentially.

The result is "a lot more potentially interesting space to explore" to find a solution, Martin says.

Martin is applying uncertainty quantification to seismic wave propagation. How these waves reflect off underground strata of earth, rock and fluids helps geologists understand just what's underground, such as oil, gas and mineral deposits.

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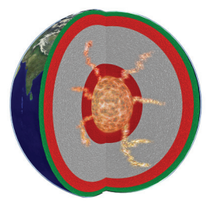
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With seismic wave propagation, Martin is trying to get at the stiffness of earth and rock layers.

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"You can think of all the Earth models that are like the true one and as you up the dimensionality, the proportion of models like yours becomes smaller and smaller," he adds. To find the correct one, "you have to explore a huge proportion of the space or have an intelligent way to go after the most interesting space."

The curse of dimensionality means even the most powerful computers can't handle many such problems. And seismic wave propagation is a notoriously high-dimensional inverse problem.

During his practicum, Martin worked on ways to construct a "low-rank subspace" — to reduce dimensionality, making the uncertainty quantification problem easier to solve.

Youssef Marzouk, who supervised Martin during the practicum at Sandia National Laboratories in Livermore, California, puts it another way. Researchers must confront an enormous number of factors influencing seismic wave propagation and other phenomena. The most naïve way to attack such problems is to attempt to capture all potentially relevant factors — sacrificing computational tractability in the process.

KNOCKING DOWN DIMENSIONS

"That's not the inherent dimensionality of the problem," continues Marzouk, who now is a professor at the Massachusetts Institute of Technology. "There are a lot of things you don't need, and with limited data and noise there are things you are never going to be able to infer." The question is "How do you distinguish the things you are going to be able to infer from the things you aren't going to be able to infer or don't need to infer?"

Martin and Marzouk use Bayesian inference to attack inverse problems. Bayesian methods make a prediction about the probability a hypothesis is true, then repeatedly update the probability distribution as more data come in.

"What we came up with … was that the interesting modes — the things we really care about — are the ones that change the most" as the Bayesian distribution is updated, Martin says.

Marzouk adds, "There are certain modes that aren't going to change much because your data … have little to say about these modes. … Those are dimensions we want to take out of the problem.

"We're trying to expose the intrinsic low dimensionality of the problem, where that low dimension combines the properties of the prior information, the data you actually observe and the physics of the forward model."

With a tractable problem, the researchers then use other techniques — like Martin's specialty, the Markov chain Monte Carlo (MCMC) method, or Marzouk's favorite, polynomial chaos expansions — to quantify uncertainty in the approximation.

Besides using seismic data, Martin and Marzouk spent much of the summer testing the technique on "deconvolution" problems. They applied a mathematical formula or kernel to "blur" a randomly generated input signal. They then used information from the blurred signal to seek the original.

Martin and Marzouk found their technique worked well on linear problems. Deconvolution allowed them to test nonlinear problems — an area in which the two continue to collaborate.

"We know how to approximate the model in a handful of dimensions," Marzouk says. "We haven't yet mated James' work with adaptive approximations of the forward model, but that will provide an additional level of payoff."

Martin and Marzouk presented their results in separate talks at the March 2009 Society for Industrial and Applied Mathematics Conference on Computational Science and Engineering, and Marzouk visited Texas in summer 2009. The two hope to generate a paper on the method as soon as they can extend it to certain nonlinear problems.

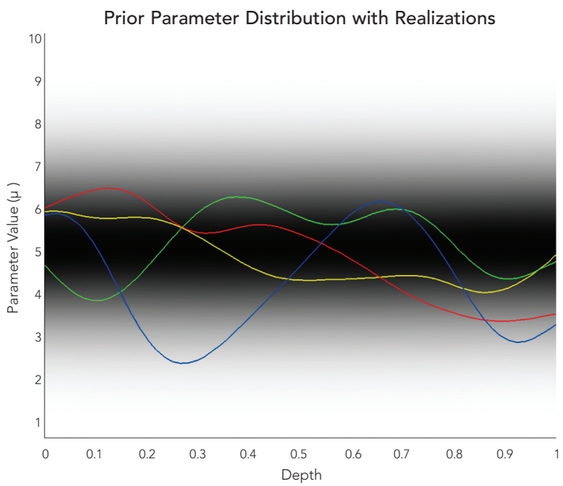
Having Martin for the summer "was just a fantastic experience," Marzouk adds. He and Ghattas, Martin's advisor at Texas, hadn't collaborated before; now they're working together on a project "and James is a key part of the mix."

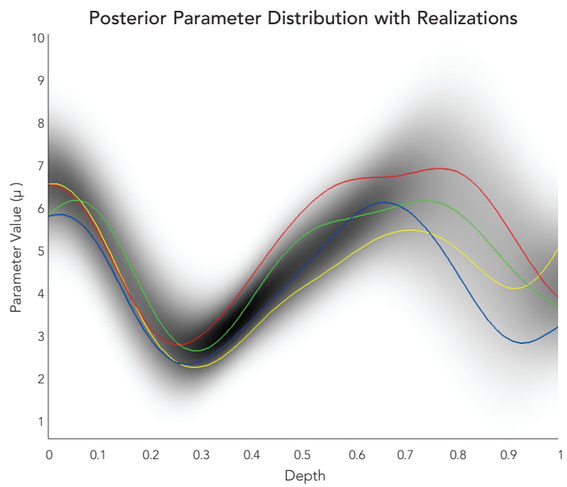
"Hopefully we'll have a longer relationship," Marzouk continues. "This problem is of interest to both of us. We're going at it from complementary directions and this core of dimensionality is relevant to both."

So relevant, in fact, that Martin's practicum experience had an impact on his doctoral research. The subject is seismic data, but the methods he uses could be applicable to a variety of inverse problems, including electromagnetic wave scattering and image reconstruction.

With seismic wave propagation, Martin is trying to get at the stiffness of earth and rock layers. In a deterministic inverse approach, scientists calculate the set of stiffness parameters that best fit observations.

"You capture the model that best accounts for your data but it's very unlikely the true model looks exactly like that best-fit possibility," Martin says. "If you want to have some kind of fault tolerance … you need to know the possible ways it can differ from the best-fit scenarios. There may be features that are completely undefined in the best fit but are not unlikely, and you would want to know about them." Those features may include oil, gas or mineral deposits.





These images depict marginalized probability distributions for uncertain seismic model parameters. The gray areas represent the probability density for the parameters; the darker the gray, the more likely it is that the parameter curve passes through that point. The blue curve represents the ground truth parameters used to generate the synthetic data. The other colored curves are representative samples from the prior and posterior distributions. The prior distribution describes researchers' knowledge of the parameter values before considering any measurement data. The prior in this case assigns high probability to parameters with an average value of 5 and without spikes or sharp boundaries between layers. The researchers use Bayesian methods to incorporate measurement data and arrive at the posterior distribution. The difference between prior and posterior distributions shows what researchers have learned about the parameters by including the measurements. It shows an improvement in knowledge about parameters down to a depth of about 0.4, since the probability is darker and concentrated in a narrow band at these depths. Parameters are more uncertain at depths from 0.7 to 1.0, which are farther from the surface and therefore more difficult to infer.
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PARAMETERS AND PROPOSALS

Statistical inverse problems generate a probability distribution for potential parameter choices. Scientists get a spectrum of answers.

"Many different choices of parameters can give you the same observation," Ghattas says, "so instead of picking just one we try to statistically estimate and assign probabilities."

Martin adds: "They can say both the things you really do know, with this degree of certainty, (and) the things you don't know."

The statistical inverse approach is a relatively new research area, Ghattas says. "The big goal is to apply it to large-scale problems."

The MCMC method Martin uses to attack statistical inverse problems samples a proposed probability distribution. The distribution is updated as each sample is tested against the true distribution. The samples are chosen at random, but in an "intelligent" way, based on derivative information from the problem.

This is where Martin and Ghattas are making some unusual tweaks. "The novel thing we're trying to do is tune the proposal distribution to reflect the actual distribution," making the algorithm more efficient, Martin says. "Hopefully, this will allow us to effectively draw samples from the true distribution."

If the proposal distribution can be tuned correctly, it will effectively result in a low-rank subspace.

"This kind of proposal distribution should be a good approximation of what's really there," Martin adds. "If that's the case then the number of samples for MCMC to converge and reach a solution shouldn't vary with dimension."

Although his goal is to avoid explicitly reducing dimensions of the problem, the technique Martin worked on at Sandia did come into play in his doctoral project. His solution requires computing the Hessian of the forward model as a way of tuning the proposal distribution. "That is, traditionally, a very expensive thing" computationally, he adds.

Martin found the linear dimension-reduction problem he tackled over the summer is closely related to finding the low-rank subspace for the Hessian. He reordered some terms in his algorithm to incorporate it.

Ghattas says that shows "It was the ideal sort of practicum." Martin "got exposed to a new environment, a new scientist in Youssef, and a different class of techniques, but the ideas and techniques he developed there have direct application" to his doctoral project.

Martin hopes to graduate in 2011 and soon will take a big step toward that goal: outlining a proposed research subject.

That's where the big thinking comes in.

"I'd like to do the seismic inverse problem with real seismic data on the entire globe," Martin says. "That would be a monumental number of parameters. If we can do it, it would be really fascinating scientific research. We can describe what's underground with some certainty."

One thing truly is certain: Martin's future is bright.

Martin found the linear dimension-reduction problem he tackled over the summer is closely related to finding the low-rank subspace for the Hessian. He reordered some terms in his algorithm to incorporate it.

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Attenuators are regulatory sequences that halt gene transcription in bacteria and other prokaryotes. If they succeed, the researchers will have a standardized tool that could provide fine-grained gene expression control.

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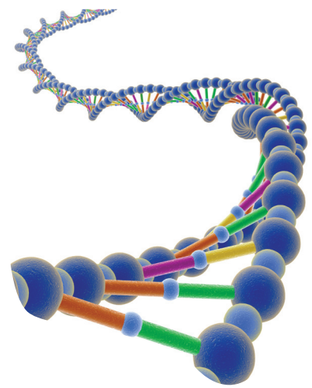

PRACTICUM SENDS FELLOW BACK TO THE BENCH

SARAH RICHARDSON
Johns Hopkins University School of Medicine
Lawrence Berkeley National Laboratory

SARAH RICHARDSON STRUCK an unusual deal with Adam Arkin before completing a practicum in his group at Lawrence Berkeley National Laboratory in summer 2008.

Richardson, a Department of Energy Computational Science Graduate Fellowship recipient, spent much of her high school and college years getting her hands wet in biology labs at Johns Hopkins University School of Medicine. But since becoming a doctoral candidate in human genetics and molecular biology at the same school, she's mostly worked with computers, devising software for gene design and for tracking synthetic yeast genome research.

Richardson missed the smells and sensations of the lab. "You can get the computer to tell you whatever you want, but you can't prove it until you go to the bench," she says. "You really have to keep both of them together."

So she asked Arkin, head of Berkeley Lab's Synthetic Biology, Physical Biosciences Division, if she could split her summer between computational work and time in the wet lab. He agreed, and Richardson's eagerness to return to pipetting and running gels became a running joke. She gratefully took on even the most mundane tasks — like washing test tubes.

"It was kind of pathetic," Richardson laughs.

Pathetic or not, she made important contributions to Arkin's research into an RNA-based transcription attenuator found in *Staphylococcus aureus*. Attenuators are regulatory sequences that halt gene transcription in bacteria and other prokaryotes. If they succeed, the researchers will have a standardized tool that could provide fine-grained gene expression control.

"This RNA-regulated attenuator provides an opportunity to, for one, engineer it for better function so it really is an off switch and has a large dynamic range," Arkin says. Since it's an antisense-mediated circuit — one that blocks transcription — engineered attenuators might be built into a family of parts operating similarly but orthogonally — without interfering with other functions — in cells, Arkin says.

Richardson describes attenuators as having two pieces, like a lock and key. Arkin's group wants to modify them so a specific lock works only with a particular key. Two or more could be inserted in the same transcript, working together much like a logic circuit.

"Think of it as a uniform framework for scalable control of gene expression, making it more like electronics than it is now," Arkin adds.

Richardson's practicum focused on improving and augmenting existing computer code to generate new attenuators orthogonal to "wild type" *S. aureus*. Under postdoctoral researcher Julius Lucks and graduate student Stanley Qi, she learned the Python programming language and wrote an interface between the group's existing code and the

She's creating algorithms to break the target genome into oligonucelotides — DNA chunks 60 base pairs long.

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Vienna RNA Package — software designed to predict and compare RNA secondary structures. The tweaks made it possible to interchange Vienna with mFold, another RNA secondary structure prediction package, and to compare the two programs' predictions.

The group's code starts with the wild-type lock and key and then mutates it, Richardson says. She devised an algorithm to choose a large set of mutually orthogonal or nonorthogonal attenuators from the mutants. The tool could help the group achieve its goal of composability — the potential to chain or stack attenuators to control gene expression.

With a list of predicted orthogons, Richardson headed to the wet lab.

"It went as you can expect a wet lab to go, which is not well," she says. It took her the rest of the summer to troubleshoot a cloning technique and devise a lab protocol.

GOING FOR THE GLYPHS

Another of Richardson's projects had a more immediate impact. The group had used a sequence-editing program called ApE to store plasmid data, and a system of glyphs to visually track myriad plasmids in lab notebooks and experiments.

When Richardson came to Berkeley, Qi was assembling the glyphs and linking the two programs by hand. "Whenever I see someone doing something by hand, I say 'Time to automate,' " Richardson adds. Using Python, she wrote a program that reads the ApE file and generates glyphs automatically for database entry.

The program is general enough that other groups have expressed interest in it, Richardson says. She planned to continue working on it, but months later still hadn't found the time.

It's easy to understand why. Richardson's ambitious research and busy class work at Johns Hopkins would be enough to keep *two* grad students busy.

The Baltimore resident was in high school when she began working with Johns Hopkins researcher Jef Boeke, a professor of molecular biology and genetics and now director of the medical school's High Throughput Biology Center. Richardson stayed on through the summers as she earned her undergraduate degree at the University of Maryland, College Park. Her senior thesis is based on work at Johns Hopkins.

In her last year of college Richardson worked on what became GeneDesign, a Web-based program that automates construction of genes from DNA segments. For instance, GeneDesign can start with a sequence of amino acids comprising a protein and provide the sequence for a gene that encodes that protein. GeneDesign also lets users choose specific codons — trios of bases that code for particular amino acids — for specific organisms. The program also inserts restriction sites — places where enzymes can cut the DNA strand.

Since the program was published in 2006, with Richardson as the lead author, thousands of researchers from around the world have accessed it on the Web.

Despite her GeneDesign experience, Richardson loved lab work and didn't want to become "the computer person." Boeke, however, suggested she study with Joel Bader, a biomedical engineering professor who would help her learn computational biology.

Richardson has focused on automating and accelerating the Bader lab's central project: creation of a synthetic genome based on the yeast *Saccharomyces cerevisiae* — one with all unnecessary genes eliminated.

"We want to make a stable platform — a chassis for biology. Then it's up to others what they make of it" by adding genes for specific functions, such as drug or biofuel metabolism, Richardson adds.

Most minimal genome research has focused on bacteria, Bader says, but yeast is a better choice for building and testing a network to operate in eukaryotic systems. "The special twist for our project is instead of trying to come up with it on our own, we will build a genome and the organism will do it" — automatically deleting unnecessary genes, Bader says.

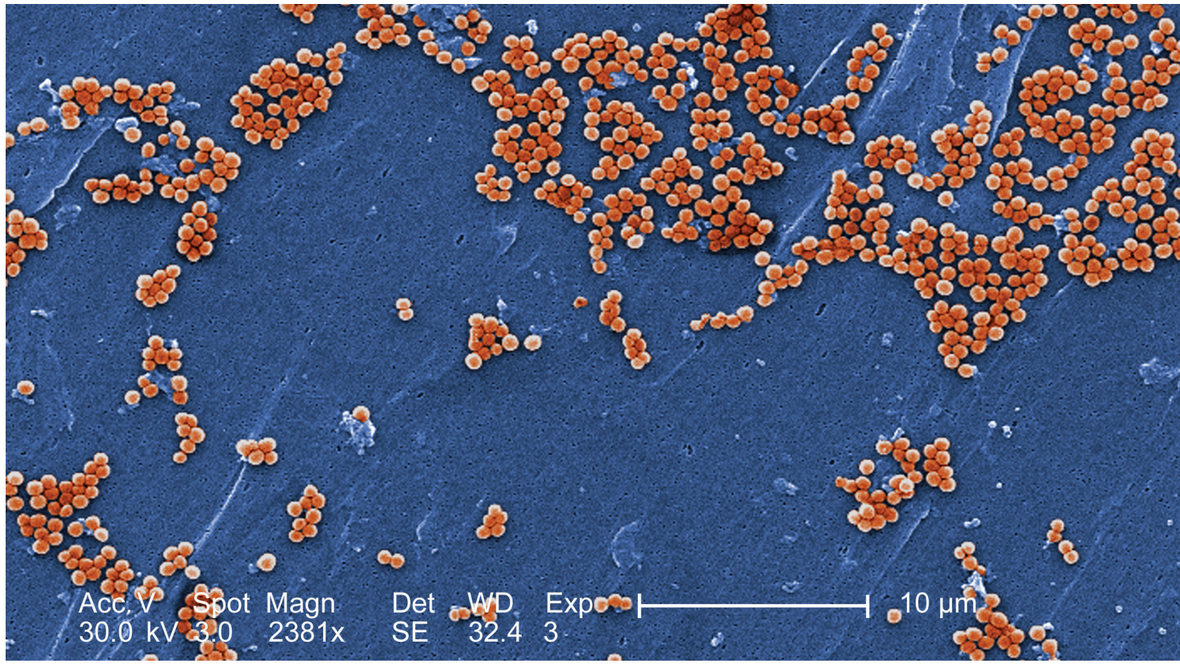
"Anything that survives on the other end is a potential answer to what is the minimal genome," Richardson says. She's creating algorithms to break the target genome into oligonucelotides — DNA chunks 60 base pairs long. Commercial labs synthesize the oligos and Johns Hopkins undergraduate students build them into bigger pieces for testing. "It's like splicing a movie together," Bader says.

Richardson's algorithms help choose designs and synthesis strategies most likely to work in the lab. Her codes also tag genes for easier tracking and predict which DNA alterations are feasible and which would conflict with design goals, Bader says.

"CONTROL Z" FOR GENOME DESIGN

Although most researchers in Richardson's group work on computers, all have wet lab counterparts — in Richardson's case, it's graduate student Jessica Dymond in Boeke's group — who puts the synthetic yeast DNA into cells.

The process is imperfect, so researchers need a way to roll back the genome design to an earlier version if there are problems. Richardson helped design a Genome Revision Control System — software that allows researchers to revert the genome to an earlier state. The program allows researchers to "check out" DNA segments, change them, and check them in to a



Clumps of a methicillin-resistant strain of *Staphylococcus aureus*, magnified 2,381 times under a scanning electron microscope. Adam Arkin's group at Lawrence Berkeley National Laboratory is studying an RNA-based transcription attenuator found in this common bacterium as a way to control gene expression.

Source: Janice Haney Carr, U.S. Centers for Disease Control
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IS THERE A "NOT A DOCTOR" IN THE HOUSE?

Sarah Richardson's e-mail address starts with "notadoctor."

It has a lot to do with her unusual position as a non-medical student in a medical school. She and other human genetics doctoral candidates at Johns Hopkins University School of Medicine are required to take two years of classes alongside future physicians.

"Johns Hopkins has the second-best med school in the country and students are keenly aware of this and proud to be here," Richardson says. It also makes some of them leery of the graduate students, especially since their priorities are slightly different.

"We're more interested in mechanisms and 'whys' and nice long philosophical discussions," Richardson says.

When Richardson found a T-shirt saying "NOT A DOCTOR" and featuring a classic image of a surgeon with a red slash across it, she figured it was a perfect way to poke fun at the students' contrasting perspectives. "Dr. Boeke asked me where I got it and I told him he couldn't have one, obviously," she jokes. The shirt became famous, faculty and family members began calling Richardson the Not A Doctor, and she changed her e-mail address.

Despite the humor, Richardson knows she's lucky to receive a first-class medical education. "One of the reasons I love this program is because they let us sit through those med school classes — and it wasn't fun and games all the time."

Of course, the e-mail name holds only until Richardson earns her doctoral degee. Her sister, who also is a graduate student, has demanded she surrender it.

"I think I'll change it to 'notarealdoctor,'" Richardson jokes.

repository for project leaders to review. The software also automates tasks such as updating genome regions affected by a new sequence.

Bader's group is assisted by what Richardson calls "our mighty undergraduate army" — Johns Hopkins students in a "Build-a-Genome" course she helped create. Students learn lab procedures and assemble DNA the researchers can study and piece together into the yeast genome.

The arrangement works well, Richardson says. Researchers get large DNA libraries at lower cost. The students earn academic credit and learn about molecular biology. "They're typically very motivated to do the work, and they get star recommendations from their professors," Richardson adds.

Richardson wrote software for the class and lectures on computer-assisted genome design each semester. In fall 2009 she — and Bader — attended every class and participated in building oligos as Richardson wrote a database program to track output.

Despite her reluctance to become "the computer person," Bader says Richardson is just that. The DOE CSGF "has given her great training because she's been able to really learn the fundamentals of what she's doing," compared to many computational biologists who pick up computer skills on the job. Richardson's rigorous courses in computer science and applied mathematics means she better understands the work and can contribute at a higher level, he adds.

That certainly was the case at Berkeley, Arkin says. His group still uses software Richardson helped create and much of it is essentially unchanged since her departure. Researchers even improved her lab protocol so much it's now automated.

"We invited her to join the group if she wanted to, and invited her for a postdoc," Arkin says, only half joking. Richardson was "bright, articulate, worked with a purpose and was just an incredibly nice person with no attitude whatsoever."

Richardson hopes to graduate in 2010, but the exact date is uncertain, partly because Johns Hopkins requires its human genetics graduate students to take two years of medical school (see sidebar).

After earning her degree, Richardson hopes for a position combining her devotion to both lab and computer work. One possibility is metagenomics — the analysis of all the genetics in a particular environment.

In Richardson's ideal post, that environment would be the human body. Only about 10 percent of all the genetic data humans carry with them come from the body, Richardson says. The rest is from the bacteria, fungi, yeasts and other entities that "make up the organism that walks around and calls itself a graduate student," she adds.

"They're going to need tools for that and they're going to need models," Richardson says, the words rushing from her in anticipation. "As a human geneticist, the human metagenome would be an awesome thing to study."

SHEDDING LIGHT ON NANOSCALE INTERACTIONS

JACK DESLIPPE
University of California, Berkeley
Oak Ridge National Laboratory

JACK DESLIPPE'S MANY HOBBIES include managing a Web page on his family's genealogy. He posted the information — gathered by some Quebec Deslippes — hoping others would fill in missing connections.

"It's interesting, because my name is not very common," says Deslippe, a Windsor, Ontario native and doctoral candidate in computational condensed matter theory at the University of California, Berkeley. "You can almost find everyone in the world named Deslippe. It's actually a tractable problem, unlike a lot of others."

Deslippe knows something about tractable problems and filling in the blanks. The Department of Energy Computational Science Graduate Fellow develops methods and designs simulations that help elucidate how nanomaterials interact with light at the electronic level. The problems are difficult, but the answers could lead to new uses for these exotic materials, such as capturing solar energy or generating laser beams.

Experimentalists can observe how materials absorb or emit light, but describing the underlying physical mechanisms requires complex theoretical input. Deslippe's research steps in to provide missing connections, predicting the electronic, quasiparticle and optical properties from first principles.

For example, a photon hitting a nanomaterial can create an exciton — an excited material state composed of an electron in a promoted condition and a hole left in the lower-energy state. Working with advisor Steven Louie, Deslippe has run simulations showing that in nanosystems these excitons act in ways that are very different from their behaviors in bulk semiconductors.

In those materials an electron and hole normally attract each other because of their opposite charges; but the attraction is reduced, or screened, by the other charges and decreases monotonically over distance, Louie says. Deslippe's calculations found that at certain length scales in one-dimensional nanosystems, like carbon nanotubes, "the attraction becomes much stronger than you would expect due to screening of all the other charges of the system in a peculiar way," he adds. "Instead of reducing the attraction it actually enhances the attraction of the opposite charges."

That's just one contribution Deslippe has made to the research group, Louie says. Besides the physics work, "He really is a whiz kid in terms of making our computer codes run much faster and more efficiently." Working with other researchers, Deslippe has improved by several orders of magnitude the speed and efficiency of the group's suite of codes to calculate the excited state properties of materials.

Those skills came to bear on a "bigger" problem during Deslippe's DOE CSGF practicum at Tennessee's Oak Ridge National Laboratory (ORNL) in summer 2008. Working with Fernando Reboredo, a researcher in the lab's Materials Science and Technology Division, he calculated quasiparticle and exciton energies in poly-vinyl carbazole (PVK), a polymer with potential uses in solid-state lighting and solar cells.

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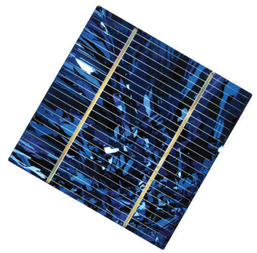
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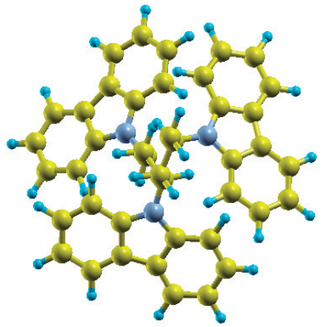
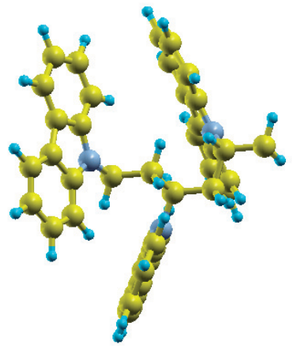




Two views of a model of a poly-vinyl carbazole (PVK) unit cell ($C_{42}H_{33}N_3$). PVK is one of the largest systems studied in the *ab initio* GW-Bethe Salpeter approach. Each contains three side groups of nearly independent molecules.

Working with Fernando Reboredo, a researcher in the lab's Materials Science and Technology Division, he calculated quasiparticle and exciton energies in poly-vinyl carbazole (PVK), a polymer with potential uses in solid-state lighting and solar cells.

PVK is known in the laboratory for its propensity to generate light under an electric current, much like a light-emitting diode. But Reboredo focuses on the material's light-absorbing qualities. It assimilates light at high energies — in the ultraviolet and violet region — and is relatively inexpensive, making it a good photovoltaic candidate.

"If you're going to use it in a solar cell it has to absorb light at the frequency of the solar spectrum, but you also have to find a way to separate the electron and hole to get the current going," Deslippe says.

BIG MOLECULE, BIG PROBLEM

The molecule's large size, at around 100 atoms, makes it a computational challenge. Reboredo and postdoctoral researcher Murilo Tiago had worked on calculating the electronic properties of PVK and similar polymers for months. Tiago's code is based on a real space density functional theory (DFT) approach — calculating the charge density of the material on a computational grid — and on using a Green's function to calculate an excited electron's energy as it evolves.

Deslippe worked with Tiago and Reboredo to combine aspects of that method with the Green's function-Bethe Salpeter equation (GW-BSE) approach that the Louie group developed and that Deslippe focuses on in his doctoral research. The researchers also are comparing their results with those obtained with the quantum Monte Carlo method, which Reboredo has used extensively.

The GW-BSE method essentially calculates the Green's function for two particles instead of one, characterizing the photo-excited state and properties of the exciton.

As he did at Berkeley, Deslippe also optimized the code to run more efficiently on an increasing number of computer processors and to calculate larger molecules. In particular, he helped implement real-space truncation — a way to limit calculations of the polymer's electrostatic interaction with neighboring polymer molecules in a supercell simulation.

All the changes paid off: The PVK system is one of the largest ever calculated using the *ab initio* GW-BSE method, Deslippe says.

The calculations showed that excitonic effects are extremely important, and Deslippe and Reboredo, working with Tiago and Louie, are continuing to study PVK's excited state spectrum. Such polymers have an unusual quality: the lowest exciton state has the electron and hole present on the same side group, while higher energy states are charge transfer excitons with the electron and hole separated from each other by an increasing distance. "When you pull the electron and hole apart, you get valid excitonic states," Deslippe says. "I think that's a good sign for these applications we're looking at."

Another Oak Ridge group, meanwhile, is planning experiments to test the simulation results.

Just as importantly, Deslippe's practicum demonstrated that the GW-BSE method could compute energies of such large molecules. That means researchers could calculate polymers' absorption spectra, band edges, work functions and exciton binding energies, perhaps leading to improved polymers for both lighting and solar cells.

Deslippe's practicum broadened his horizons, Louie says, by giving him the chance to study a class of complex materials different from the graphene and nanotube systems he researches for his dissertation. He also was exposed to different mathematical methods for calculating a material's optical properties.

THREE STEPS TRACK MANY-ELECTRON EFFECTS

Louie's group developed the GW method in the 1980s to calculate the band gap and quasiparticle energies of bulk systems like silicon from first principles. Now the researchers are combining it with the Bethe-Salpeter Equation to compute the spectroscopic properties of a variety of systems, including nanostructures.

Researchers have long known that including such effects as the electron self-energy and excitons is important for correct results, and some have tried to account for them in DFT calculations. But these attempts don't describe the many-body effects well, Deslippe says. In essence, electrons throughout the rest of the system move around to counter the new field or charge, modifying the interaction.

The GW-BSE method accounts for the many-electron effects with a computationally efficient three-step process.

First is a DFT calculation to arrive at the system's ground state properties — before electrons are excited. "In order to really design a system or nanostructure one has to determine where the atoms are," Louie explains. "What we do as a first step is to determine the ground-state geometry" and accompanying properties.

Next, the GW approach calculates the attributes and interactions of a single excited electron as it evolves. Particles added to the system "meld" with it over time, but those with a long lifetime behave almost like an independent particle, but with modified properties — a quasiparticle.

"We single out one electron being excited and look at its behavior or look at the hole left behind and see how it behaves," Louie adds. "Because it's a many-body system the electron behaves in a different way than if you were to have a noninteracting system of particles."

The last step is solving the Bethe-Salpeter equation to include the electron-hole interaction. "We single out the two particles and treat them more accurately. We ask the question of how the electron and hole interact with each other and all the other electrons in the system," Deslippe says.

The important part, Louie adds, "is we can do all the steps in the calculation without any empirical input. We do it from first principles."

Deslippe and Louie, working with others, have applied the GW-BSE technique to a number of systems. In one paper they describe calculations of excitonic effects in graphene. Because of its semi-metallic nature, graphene might be expected to show little electron-hole interaction since the freely moving electrons around them would have screened the effect.

But the calculations found a surprisingly large excitonic effect in graphene — a shift of the prominent peak in the optical absorption spectra of 600 milli-electron volts (meV), from 5.2 eV to 4.6 eV. "Bound exciton states can even be found in metallic nanotubes, where one would expect the interaction to be very weak due to screening," Deslippe says. That raises hopes that graphene could also be tunable for use in tiny opto-electronic devices.

Deslippe's contributions have been vital to achieving such results, Louie says. When the group first began studying nanomaterials it could only model small structures. Thanks in part to Deslippe's work, "We're now able to look at nanostructures and periodic systems with unit cells that have hundreds of atoms. That's a major advance."

Deslippe and Louie plan to extend their methods to higher-order optical and electronic effects — calculating the effects of multiple photon absorption and the coupling of the exciton with lattice vibrations to get a more complete picture of a material's absorption characteristics.

"You can explore different systems and even create artificial, yet-to-be-made systems," Louie says. "Then hopefully you can tell the experimentalists what to make."

Deslippe also is working to make the code even more efficient and user-friendly for other researchers. "Frankly speaking, we have one of the most efficient computer codes for these kinds of first-principles studies."

Meanwhile, Deslippe, Reboredo, Louie and others are composing a paper describing PVK's physical properties regarding photovoltaic and solid-state light applications.

"It's great to get to work with people who are experts in related subjects, but not the type of subject you would get" working in the research group at Berkeley, Deslippe says. He also learned by getting to know researchers throughout the lab, from theoreticians to experimentalists.

Deslippe is getting set to graduate. After that, he's unsure whether he'll work in a national laboratory, academic or corporate setting. But he's sure of one thing: "I'm definitely trying to do research in some environment."

ALUMNI PROFILES

GRADUATES NOTCH ACHIEVEMENTS

Researcher Tunes Into Networks

MICHAEL WU has the training of a statistician, an applied mathematician and a computational neuroscientist, but what he does may have just as much in common with psychology and sociology.

As principal scientist of analytics at Lithium Technologies Inc. in Emeryville, Calif., Wu studies on-line communities and the interactions within them. Lithium provides software and services that let companies use these and other social media to serve and understand customers. If done right, Wu says, social media create user communities that supplement a firm's product support, provide instant product feedback and turn customers into advocates.

"A lot of companies are afraid of this social revolution because in some ways they lose control of their customers or their brand. People can say whatever they want," adds Wu, a Department of Energy Computational Science Graduate Fellow at the University of California, Berkeley, from 2002 to 2006. But social media also help companies boost sales through word-of-mouth advertising, and product innovation through idea exchange.

Lithium, whose clients include AT&T, MTV Networks and Barnes & Noble bookstores, has a wealth of customer conversation data from hundreds of communities, Wu says. That gives him plenty of fodder for detecting trends and testing approaches.

One of Wu's research projects focused on the role of customer networks in word-of-mouth marketing. Using anonymized data from several Lithium communities, he developed an agent-based modeling technique to simulate the random diffusion of information across the customer network. Among other things, Wu found that targeting specific influential users made word-of-mouth programs more effective and less expensive; 80 percent of the potential value came from targeting less than 5 percent of the potential audience.

Wu's current research concentrates on understanding two classes of users at opposite ends of the spectrum: superusers, who contribute heavily to forums and interact regularly with others, and lurkers, who visit forums for information but never contribute.

Wu hopes to get at what motivates superusers and how they emerge, and at what predicts who will become one. "Why do they do what they do? … Aside from the virtual psychological benefit (of helping others), they don't seem to get a lot."

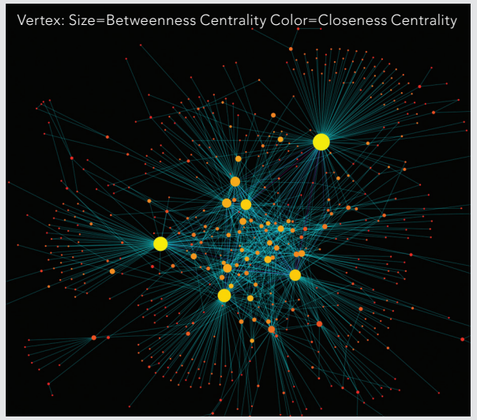
The goal is similar for lurkers: understanding what keeps them engaged without participating, how to bring them into the conversation, and even how to coax them into becoming superusers themselves.

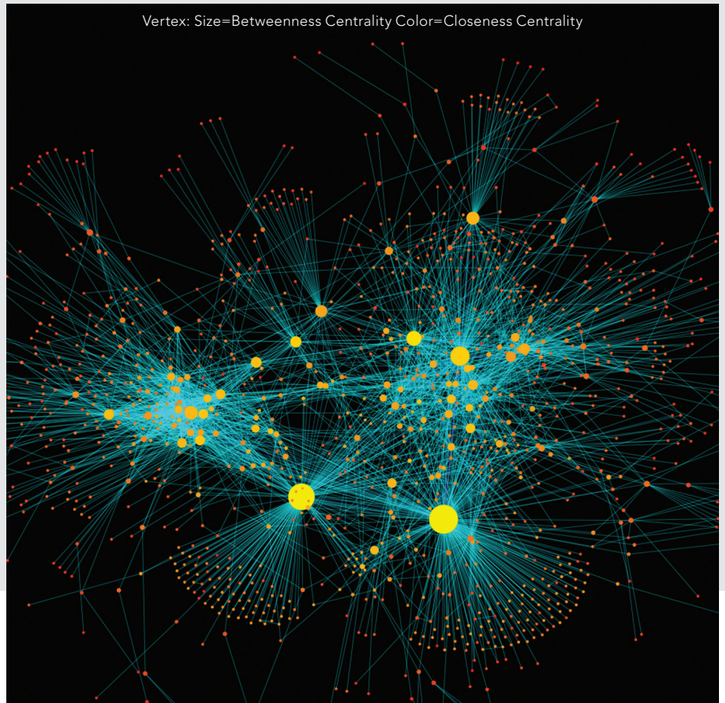
Turning both kinds of users into business assets involves a lot of psychology, Wu says. "Incentives, rewards, ranking systems, gaming dynamics and serendipity all play important roles in managing and maintaining a successful community."

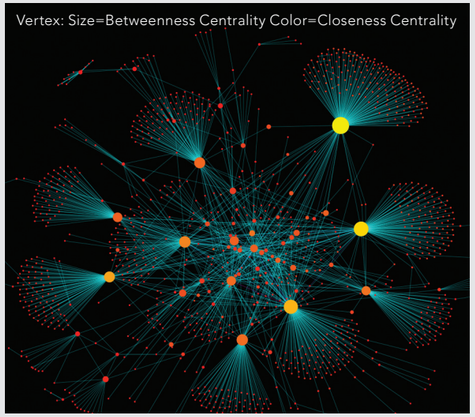
Such communities could revolutionize business, Wu says, by giving customers an effective channel to voice opinions, and giving companies an efficient way to listen. That makes companies more responsive to consumer complaints and needs.

Riding the revolution appeals to Wu. Though his 2008 doctoral work is in computational neuroscience, he's drawn to the complex, fascinating interactions that drive social media. The abundance of data and the fast pace of the business world, he says, lets him test hypotheses and apply solutions more quickly than in a laboratory or academic setting.

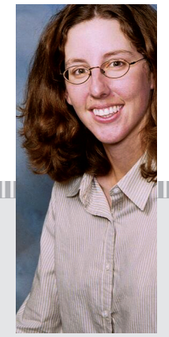
"We focus on real-world problems that are very practical and in some ways messier — there usually are a lot of constraints and we must constantly make trade-offs between time to market and the quality of the solution, or between efficiency and accuracy of the solution," Wu adds. Yet, "In the business world I feel I can actually make a difference faster, and not just when I'm 80 years old."







As principal scientist of analytics at Lithium Technologies, Michael Wu uses anonymized data to generate thousands of social graphs like these to understand the interactions in on-line user communities and how they evolve. The lines represent interactions between pairs of users, which are represented by the dots. The size and color of the dots represent a user's importance and influence.



Speaking Many Languages

WHEN STRANGERS ASK WHAT she does, Judith Hill has an initial straightforward answer: She's a computational scientist.

"They may say, 'What's that?' Then I say I'm part engineer, part mathematician and part computer scientist all rolled up into one," adds Hill, a researcher in the Computational Math Group at Oak Ridge National Laboratory in Tennessee.

The combination appeals to Hill, who held a Department of Energy Computational Science Graduate Fellowship from 1999 through 2003. "I view myself as a communicator, so I like sitting at the intersection of several disciplines," she says. "Applied mathematics allows me to communicate with mathematicians, computer scientists and domain specialists. I can speak a lot of different languages and bring in new ideas they may not have thought of."

Hill's first and perhaps best "language" is fluid dynamics. Her doctoral research at Carnegie Mellon University laid the foundation for modeling how red blood cells are deformed and damaged as they flow through an implanted pump designed to assist a failing heart.

She expanded her mathematical vocabulary in the Applied Math and Applications Department at Sandia National Laboratories' New Mexico location from 2005 to 2008. She focused on solving inverse problems, a class of optimization problems, that were constrained by a physical model represented by a set of partial differential equations (PDEs). In inverse problems the value of some model parameter is inferred from observations or measured data the parameter produces.

"A lot of researchers in the field of optimization work on discrete problems. The work I do is in continuous problems," Hill says. Solutions could be any number in a range rather than distinct separated values. "The solution space we're looking in can be a lot larger than many traditional optimization problems, thus requiring large computers to become computationally tractable."

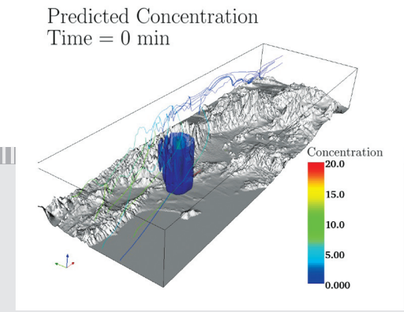
Inverse problems drew her attention, Hill says, because they offer a rare glimpse at an end use for her work. "In applied math, the direct use of our work in real-world applications can be many years away, because we're working on new and unproven methods and techniques."

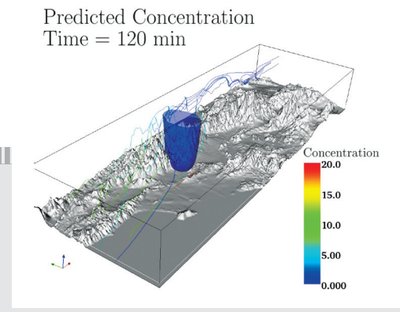
In one case, Hill and her colleagues calculated a test problem tracking the spread of an airborne contaminant in the Los Angeles area to its source. Such models are important for planning emergency responses, monitoring public health, assessing hazards and other functions.

Hill has returned to fluid dynamics since moving to Oak Ridge in 2008, but with a different tack. Instead of focusing on finite elements methods, a classical numerical technique that was her main approach, she's working within the MADNESS framework.

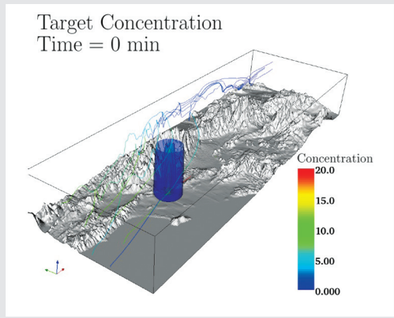
Developed by researchers from Oak Ridge and the University of Colorado, MADNESS stands for Multiresolution Adaptive Numerical Scientific Simulation. It relies on multiwavelets, a method treating regions of space with different degrees of accuracy, to calculate things like fluid flow and molecular electronic structure. The method approximates some problems more accurately than other techniques, Hill says.

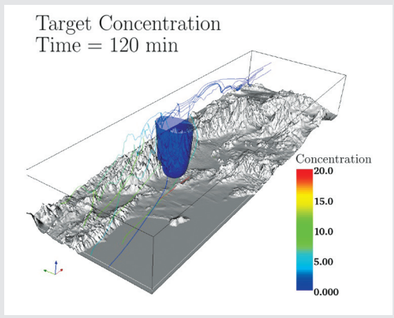
The other major element in Hill's research is tuning algorithms to run well on massively parallel computers. It's an especially challenging job these days, she says, as designers move from merely adding processors to creating hybrid machines with combinations of chip architectures.





These visualizations show the solution of an inverse problem characterizing the spread of a simulated airborne contaminant plume in the Greater Los Angeles basin. The inverse problem was calculated based on measurements synthesized by solving the convection-diffusion equation using the target initial conditions and recording measurements on a 21 by 21 by 21 uniform array of sensors. Compare the predicted concentrations from solving the inverse problem at zero minutes elapsed time and after 120 minutes with the target concentrations at the same times.





Hill is in a good place to test her approaches at Oak Ridge, home to powerful machines like Jaguar, rated in 2009 as the world's fastest computer. That, the lab's growth and the mountainous eastern Tennessee region all attracted her, she says.

A laboratory environment also offers a balance of things she loves most about research, Hill adds. "I really enjoy mentoring students and postdocs, and within the lab we have the opportunity to do that." And unlike a university, where professors often are walled-off from colleagues in other disciplines, at Oak Ridge Hill has opportunities to fulfill her favorite role as scientific liaison.

"I view the role of a computational scientist as a builder putting together the many pieces required by computer simulations to get science done. These pieces include developing new physical models, improving numerical techniques and ultimately developing the software for these simulations," she says. "Most of all, I enjoy working with my colleagues in other disciplines to solve problems."

Wilkening Wades Into Fluid Situations

IT'S NATURAL that fluids fascinate Jon Wilkening. As a competitive swimmer, he's spent a lot of time struggling through the world's most ubiquitous liquid.

"I think about fluid mechanics a lot while I'm swimming," says Wilkening, a Department of Energy Computational Science Graduate Fellow at the University of California, Berkeley, from 1997 through 2001 and the 2003 Frederick A. Howes Scholar in Computational Science. Nonetheless, "It's hard to figure out how to turn that into something you can use to go faster."

Fluid mechanics are a theme in Wilkening's work, but his interests range widely, as befits an academic who goes wherever interesting problems lead him. He's researched lubrication theory, microchip failure, stress singularities in solid mechanics, shape optimization and other subjects as a postdoctoral fellow at New York University's Courant Institute and, since 2005, as an assistant professor of mathematics back at UC-Berkeley.

Many of these applications tie into Wilkening's current interest in time-periodic solutions of partial differential equations (PDEs).

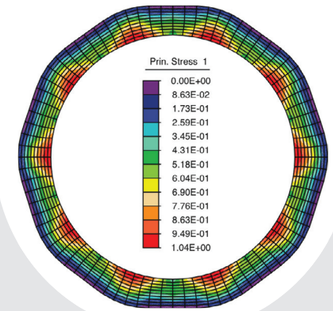
Time-periodic solutions are useful for modeling systems that reset themselves, such as ocean waves, Wilkening says. "If you can set the system going so that it later comes back to where it started, the solution will repeat itself forever." These solutions "tell you a lot about the system, going beyond what you can get from studying traveling waves, for example."

That makes time-periodic solutions good for attacking some interesting problems, Wilkening adds. In one proposed project, he and UC-Berkeley Civil Engineering Professor Sanjay Govindjee take on tires.

"When a tire is rolling, it's a system that is inherently periodic," Wilkening says, resetting itself with each rotation. Methods are available to model smooth tires effectively, but "as soon as you put a tread on it, they don't know what to do next. They don't know how to model it."

Wilkening and Govindjee believe their time-periodic methods can capture the dynamic behavior of tires between each touchdown of regularly spaced treads onto a surface. If they're successful, their research could enable faster, cheaper prototyping to make tires more safe and durable.

This two-dimensional simulation models a rubber wheel with an inner radius of 8 mm and outer radius of 10 mm, spinning at 955 Hz and pressed 0.1 mm onto a frictionless plane. The image shows a bifurcated deformation state, exhibiting standing waves, and first principal stress contours (N/mm^2).



Wilkening and David M. Ambrose of Drexel University used similar methods to tackle an seemingly unrelated problem: computing time-periodic vortex sheets with surface tension. A vortex sheet, as they describe it in a paper accepted for publication in the Proceedings of the National Academy of Sciences in 2010, is the interface between two fluids as they shear past each other. Prior to their research, it was not known whether time-periodic solutions exist.

"It's a really interesting application for the algorithm I have for finding periodic solutions," adds Wilkening, who received a 2010 National Science Foundation CAREER award for a proposal entitled "Optimization and Continuation Methods in Fluid Mechanics." "What we're bringing to the table are numerical methods that can answer some very difficult analysis questions."

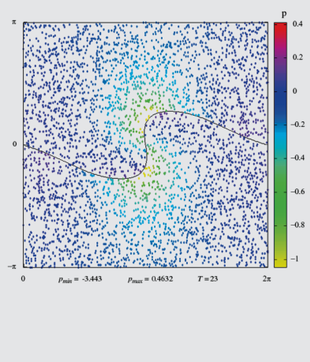
The key, he says, is finding an adjoint system that allows computation of the gradient of an objective function quickly and efficiently. For example, a swimmer may want to minimize his drag — the objective function — as he goes through the water. The first step would be to write the formula for drag in terms of the solution of the Navier-Stokes equations. "There's another PDE related to Navier-Stokes, the adjoint PDE, that tells you how the drag will change if you change your stroke," Wilkening says. "Solving the adjoint PDE tells you the best way to swim faster."

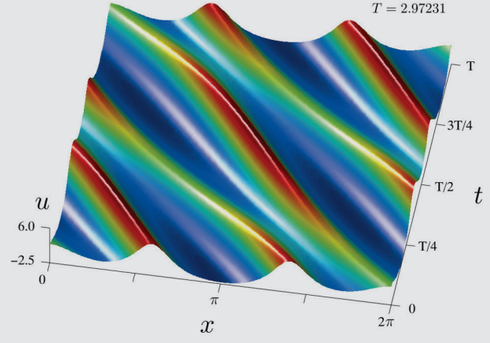
In their paper, Ambrose and Wilkening use similar adjoint techniques to compute families of smooth, symmetric "breathers" — oscillatory nonlinear waves — that alternate between a flat state of maximum kinetic energy and a rest state with all the energy stored as potential energy in the interface. In some cases the interface overturns before returning to the initial, flat configuration, the paper says.

Wilkening has settled into academia, a place he loves for the opportunities to work with students and pursue interesting research, but it wasn't a goal. "I thought I would be an engineer in high school. It wasn't until college, when I started taking advanced physics and math courses, that I realized one could actually be a professor."

Now, "I enjoy answering the hard questions you can't answer without simulation," particularly those involving complicated physics. Plus, "I've had a knack for coding my whole life. It's good to do things you're good at."

This snapshot from an animation shows a time-periodic solution of a vortex sheet with surface tension, with the interface exhibiting a "breather" pattern of oscillatory nonlinear waves. The interface turns over before returning to its initial flat state. The particles are added for visualization and are color coded by pressure. To see the full animation, go to *http://math.berkeley.edu/~wilken/vtxs3.html*.





This image shows a time-periodic solution of the Benjamin-Ono equation over one spatial and temporal period. The Benjamin-Ono equation is a nonlinear, nonlocal, dispersive equation that models internal waves in a deep stratified fluid (such as the ocean) in certain asymptotic limits. Ambrose and Wilkening used their numerical method to compute families of time-periodic solutions connecting pairs of traveling waves through bifurcation.

WINNING ESSAYS

ENCOURAGING COMMUNICATION THROUGH ANNUAL WRITING CONTEST

WINNER

WHY DON'T BATTERIES IMPROVE LIKE TRANSISTORS?

(And what a billion transistors can do about it)

by Anubhav Jain

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.

SOMETIMES I TRY to do too much at once. Recently, as I devoured my lunch while reading e-mail on my laptop, I attempted to open a water bottle with my free hand. I succeeded — only to subsequently shower the laptop in spring water. It would never display e-mail again.

Still, I took comfort that my laptop had lived a full existence, reaching the ripe old age of three years. Most laptops currently on the market could easily compute circles around my old friend. Nearly every major component of modern laptops — the CPU, RAM, hard drive, and even the tiny onboard camera — becomes outdated in a few years.

I emphasize *nearly* everything because the battery is a holdout; since the 1990s, laptop batteries have comfortably thrown in the towel after about four hours of operating time. Slate.com journalist Farhad Manjoo jokes, "What we know about batteries today is pretty much what we knew about batteries back when ENIAC [the first computer, created in 1946] was invented." Although Manjoo's statement is technically incorrect, his point remains clear: batteries simply don't improve at the same pace as other computer components. My goal is to turn this problem on its head by *using* the stunning improvements made to CPUs, RAM, and magnetic storage to rapidly advance battery science.

But first things first: Materials researchers would argue that battery storage capacity steadily improves (about 8 percent a year), but consumer electronics producers typically offset these gains by introducing power-hungry processors or using smaller battery packs, thereby keeping the total battery life constant. While these 8 percent gains might be noticeable to a materials engineer, they don't hold a candle to Moore's law, which states that the density of transistors (the individual logic components of a computer processor) on CPUs doubles every two years.

To better understand this contrast, we can examine "Bringing New Materials to Market," a February 1995 Technology Review article. Written by Thomas Eagar, former head of the Department of Materials Science and Engineering at MIT, it demonstrates that *any* new materials technology, whether Teflon or titanium, takes about 18 years to progress from lab to consumer use. Eighteen years is an eon in the world of technology, equivalent to the time it took to leap from creating the first IBM PC to having Google in 10 languages. Transistors skirt "Eagar's 18-year law" because their basic materials largely stay the same while their design improves. Like a musician who learns a difficult passage by first playing it slowly, then gradually increasing the tempo, computer engineers have designed today's miniscule transistors by first building large ones, then making them progressively smaller.

So why do materials-driven technologies like batteries stagnate in the lab? Eagar points to the problem of *simultaneous optimization:* new materials must pass through several difficult, often-overlapping hoops to become viable products. Like a potential new headache medicine that soothes pain more quickly but may also increase the risk of stroke, a new battery material might boost operating time but degrade with use or burst into flames when overheated. When promising new materials are found, years or even decades can be spent engineering cures to their undesirable "side effects."

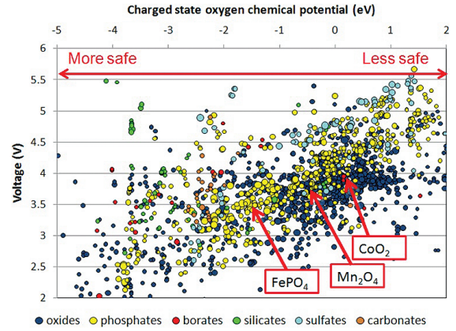
Simultaneous optimization is time-consuming because each data point can take days, weeks, or even months to collect. However, computational materials science can break Eagar's law by using theoretical calculations to model material properties. Computational materials science is now so advanced it can predict many of a material's characteristics nearly as accurately as lab measurements.

It also presents several advantages over experimental lab work. For one, computers can work around the clock without coffee breaks (unlike scientists). And, because transistors, RAM and magnetic hard drives have greatly improved, one dollar's worth of computing power today is equivalent to hundreds of thousands of dollars worth from 20 years ago. Nowadays, even a moderate research budget can purchase hundreds of powerful computers to work like a virtual army of lab hands testing endless combinations of materials chemistries. Called high-throughput computational screening, this new technique has the potential to discover and optimize new materials in record-breaking time. My colleagues and I have used Density Functional Theory calculations, some of the most accurate techniques for modeling materials, to create the world's largest computational screening endeavor. Though the details are abstruse, such calculations achieve their accuracy by using the principles of quantum mechanics to predict a desired material property.

Using our method, we've screened more than 20,000 materials as we search for a lightweight, compact battery cathode that quickly absorbs lithium during discharge and releases it safely when charged. Such a material could revolutionize electric vehicles or grid-level power storage. (And it will allow you to watch that second DVD on long plane rides!) Each potential battery material was evaluated as a whole — not only for its ability to store a lot of energy but also for its potential safety, stability, performance, cost and toxicity. Because each candidate passes through several optimization hurdles before time-consuming (and expensive) lab work even begins, commercialization can come much quicker than materials discovered without this pre-screening advantage.

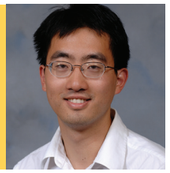
In the high-throughput battery cathode project, we have predicted several new and promising materials for use in next-generation batteries. These materials were recently made and tested in the lab and exhibit good performance.

Meanwhile, our computing clusters containing a billion transistors are busy doing a whole lot at once, computing thousands of additional chemical combinations in search of the next breakthrough battery material. Fortunately, they aren't juggling bottles of water.



Each point in this graphic represents one material, with the point size representing the material's stability. The graph shows there is a tradeoff between the voltage of a potential new battery material and its safety. High-voltage materials have better energy densities but generally are less safe. Experimental data, represented by the three points shown, suggest this trend but are unable to confirm it. The plot also shows that safety varies widely by chemistry. Oxides, which are the best-studied cathode materials, are the least safe for a given voltage. Up-and-coming chemistries like silicates demonstrate better safety, suggesting they are fertile territory for more investigation.

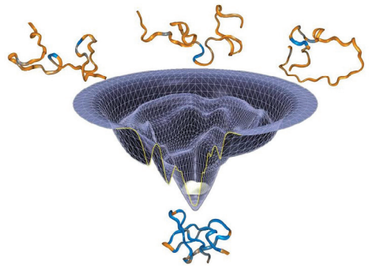
HONORABLE MENTION



UNDER THE HOOD

Predicting Proteins with Computers

by Milo Lin



The energy landscape, which plots the energy of a protein as a function of its structure, helps represent the protein folding process. Starting from a random shape, or conformation, the protein will change until it reaches the lowest energy (i.e., native) fold, which is at the bottom of the funnel in the energy landscape.

WE ARE TAUGHT that cells are the building blocks of life, so the words "biological complexity" usually conjure up images of bacteria colonies or the human brain. Yet if we were to think about cells as more than just black boxes, we would see that the mystery of life starts within them. When the cell is magnified a hundred million times, life is revealed to be the net result of molecular machines at work — machines called proteins. Proteins are the cleaners, builders, motors, messengers and transporters of the cell. Just as a car runs as a result of cooperation between many smaller components, the cell's vitality arises from the cooperative actions of proteins. So how proteins are manufactured into such a rich array of moving parts is a basic biological question.

Of course, unlike with a car, we can't simply pop the hood and look. But because we know the physics governing proteins, it's theoretically possible to predict their structures with computers. This could aid in designing proteins for use as medicines, nano-machines and specialized materials. For example, current chemotherapy drugs cannot be tailored to exactly fit the markers of cancerous cells, leading the drug to also disrupt non-cancerous cells. If protein drugs can be designed to specifically fit the markers, chemotherapy could be drastically more effective with fewer side effects.

THE BASICS OF PROTEIN SYNTHESIS

All proteins are chains of simple molecules called amino acids. Though there are just 20 different natural amino acids, the number of possible protein sequences increases exponentially with the length of the protein. Each sequence corresponds to a structure and each structure corresponds to a function.

The particular sequence of every protein is encoded by a corresponding segment of DNA, which is stored in the nucleus of each cell in our body. When a particular protein is needed, its DNA blueprint is copied and the code translated into the matching amino acid sequence. The linear chain is then molded in three-dimensional space into the structure that will carry out the protein's particular function. Called the *native fold*, this structure is stabilized by chemical forces both within the protein and between the protein and its surrounding environment (mostly water).

PROTEINS: AMAZING MOLECULAR MACHINES

It's unclear just how a protein attains its native fold. Life requires proteins to be functionally reliable, so each protein sequence has evolved to have a unique shape that is more stable than all other possible folds combined.

Because native folds are highly complex and irregular, often resembling a tangled ball of yarn, their stability is one of the most awesome examples of how natural selection can lead to creations that are both fantastical and successful. It therefore came as a shock when American biochemist Christian Anfinsen discovered in the 1950s that proteins fold by themselves without the aid of any cellular machinery.

Even more amazingly, proteins can find their native folds immediately; in fact, as American molecular biologist Cyrus Levinthal noted in 1968, proteins seem to fold trillions of times faster than expected! Consider the example of a protein 100 amino acids long. If each amino acid in the chain can be in one of two positions (far fewer than the actual number of possible orientations), then there would be 2^{100} possible folds for the protein. Even if the protein could try each of those folds in a trillionth of a second, it would take about 20 billion years for it to find its native fold — longer than the age of the universe. Instead, proteins actually fold in milliseconds to seconds.

There are simple things that self-organize (freezing water) and complicated things that external machinery reliably make (airplanes). There are also many examples of complicated phenomena that non-reliably self-organize (the weather). Proteins are unique because they are complicated structures that *reliably* self-organize. In fact, they fold astronomically faster than random search. This seemingly impossible engineering feat at the molecular level is the scaffolding that allows life to be simultaneously complex and efficient.

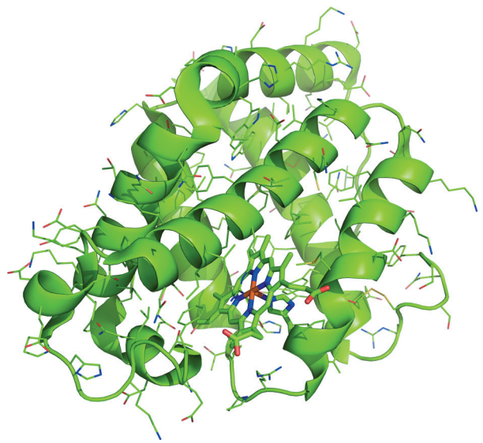
ARE PROTEIN STRUCTURES COMPUTABLE?

This complexity means computational simulation is the only theoretical tool for understanding proteins at the molecular level. In the most common approach, called molecular dynamics (MD), the simulation is broken into many small time steps. The technique calculates the forces on the protein at each time step to simulate the folding of the 3-D structure. The strengths of the many different forces are obtained from experimental data.

The protein and surrounding water molecules have uneven distributions of positive and negative charges. Since like charges repel and opposite charges attract, one of the key forces acting on the protein comes from adding up all the attraction and repulsion forces between every two atoms in the simulation. This is the calculation bottleneck in MD simulations, since the number of forces to be computed scales as the square of the number of atoms. With the total number of atoms reaching the tens of thousands even for small proteins (with water), simulations using massively parallel computing have only recently been able to span one millionth of a second.

MD simulations already demonstrate remarkable accuracy in predicting native folds for rudimentary proteins. Insights from such simulations promise to increase alongside the exponential growth of computing power, because computation holds the only promise of atomic-scale resolution. We are nearing the time when simulations can finally catch up with experiments in spanning proteins' entire folding times. When that day arrives, we will finally be able to watch as proteins transform themselves from inert chains into active machines.

Ever since microscopes first showed cells revving with vitality, the inner workings of cellular machinery have been hidden from view. Now, we are finally starting to peer under the hood of life.



Four of these subunit proteins combine to form hemoglobin, which transports oxygen and carbon dioxide through the bloodstream. Both are attached to the iron atom (shown in orange) in the heme group.

HONORABLE MENTION

SOLVING GENOMIC JIGSAWS

Piecing Together DNA With Computing Power

by Scott Clark

WHEN I WAS A CHILD I loved jigsaw puzzles. Big, small, skylines, fantasy landscapes — whatever I could get my hands on. I would sit for hours at the dining room table, meticulously building fantastic worlds piece by piece.

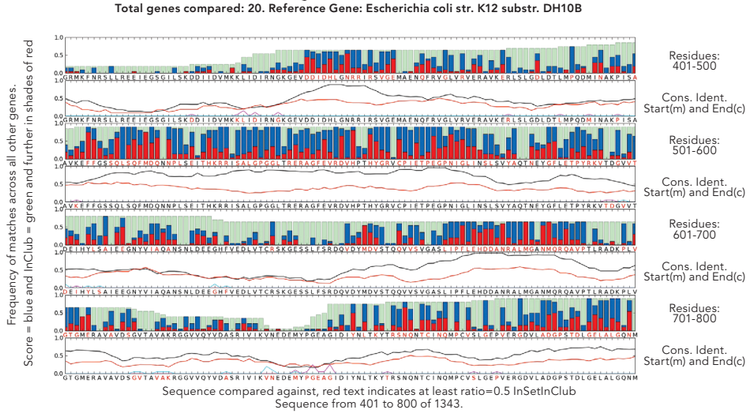
Today, I teach computers to reassemble puzzles. It's called computational metagenomic assembly, but the idea is the same. The puzzles metagenomics poses aren't traditional; each piece is a small chunk of genetic information — the DNA that comprises the universal building blocks of life.

Metagenomics deciphers all the genetic material of all the organisms in a community, like all of a person's intestinal tract bacteria. Assembling all the genetic information of viruses and organisms like bacteria into their complete genomes lets us deduce vital information about their composition and relation to each other. This can lead to new understanding of their interactions and — ultimately — vaccines to fight the viruses.

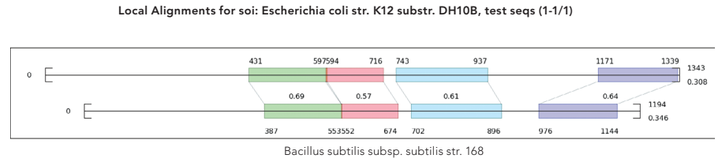
These metagenomic puzzles differ in many other ways from the puzzles I solved as a child. They are simpler in some respects; instead of an entire picture one only needs to assemble all of the pieces in a line. Unfortunately, the difficulties quickly outpace this apparent simplification. The number of pieces can easily reach the millions, if not billions, for a single assembly. Also, each piece represents only an extremely minuscule fraction of the fully assembled picture, which is usually unknown.

In metagenomics scientists also are trying to assemble many pictures concurrently, and many of the pieces may be missing while others may have multiple duplicates. "Sky pieces" — repetitive patches of blue and clouds — are the bane of any puzzler. Nature provides an equally challenging analogue, as many of the genetic pieces are virtually or actually indistinguishable. There also can be long stretches of intentionally repeated information.

Imagine taking every puzzle in a store and mixing them while making the pieces smaller, and then removing the boxes with the pictures along with a bunch of the pieces. Then try to rebuild all the puzzles to a level of accuracy that would allow you to gain information from the resulting pictures. That is metagenomic assembly.



These bar graphs illustrate alignments of DNA and amino acid sequences from multiple organisms. They show areas of high conservation, in which many organisms share particular sequences. Areas that produce high values on the bar graph are highly conserved across many sequences. That makes them likely to represent important genetic information worthy of more study.



This map of local alignments shows what parts of which genes line up and where, illustrating relative areas of conservation between two chunks of sequence data. The comparison shows which areas are conserved, which match up, and where shifts, insertions and deletions are, helping scientists understand how distantly two sequences are related on an evolutionary time line.

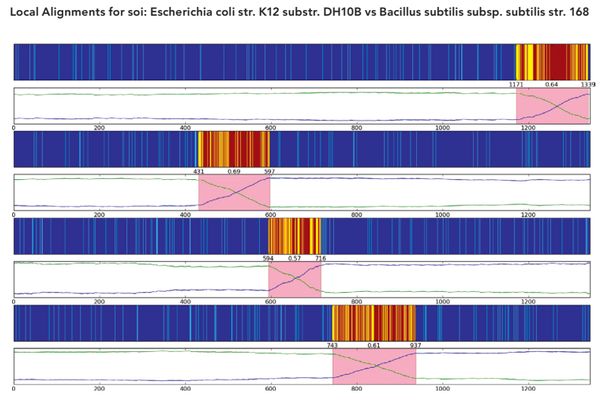
This Herculean task seems impossible at first, and normally it would be — for a human. The sheer quantity of the information to be analyzed can be on the same order of magnitude as the printed works in the Library of Congress. It would be impossible for a single person to even look at all of the pieces of this puzzle, let alone begin to assemble it.

All is not lost, however, because it's possible to train a computer to help, if you can develop a good algorithm — a specific set of rules — for it to follow. As a child, you quickly learn basic "tricks" that allow you to solve puzzles more quickly and efficiently: find the corner pieces first, build the border, put all similar pieces together, build related parts together. In much the same way, computational scientists can develop an analogous set of rules that will allow a computer to attack this problem more efficiently: find known gene pieces, find overlapping information, build from unique "seed" pieces.

Another key trick is the ability to parallelize. Modern supercomputers can process many thousands of instructions simultaneously — in parallel. Solving puzzles was always easier with a friend; similarly, these supercomputers employ thousands of processors to assemble pieces while sharing information as they go and allowing for useful information to be discovered in a reasonable time.

The field of metagenomics is still in its infancy, but scientists are sampling more microbial communities all the time, from mineshafts to human intestinal tracts, and beginning to publish results. It's still unknown what applications this research may have or the extent and ramifications of its impact.

What is certain is that supercomputers will play a vital role. By training them correctly, we can grasp this otherwise intractable task and gain a depth of understanding about the world around us. Using some of the largest computers in the world lets us solve some of the smallest and most complex puzzles in nature. This knowledge can be used to develop vaccines and better understand the composition of and interactions between living things, from the microscopic to humans. Not only is this a vital step in understanding the biological systems around us, it also gives me an excuse to keep playing with puzzles.



This shows how the computer algorithm finds areas of conservation. The top line shows where there are matches between one sequence and an offset of another. The lower line shows when the density of these matches is larger than a chosen cutoff value. This area of high density is a potential match between the two sequences and is marked off in the graph.

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
BRINGS RECOGNITION, AFFIRMATION AND RESPONSIBILITY

2010 WINNER JULIANNE CHUNG

Julianne Chung has been selected as the 2010 Howes Scholar in Computational Science. Dr. Chung was a fellow from 2006-2009. She received her Ph.D. from Emory University and is currently a NSF Mathematical Sciences Postdoctoral Research Fellow at the University of Maryland.

JEFF HITTINGER first heard of Frederick Howes a few months after starting a post-doctoral research post at Lawrence Livermore National Laboratory (LLNL) in 2000. His coworkers encouraged him to attend a March 2001 applied mathematics and computational methods conference at the nearby University of California, Berkeley, that Howes' colleagues organized in his memory.

Howes, manager of the Department of Energy's Applied Mathematical Sciences Program, died unexpectedly on Dec. 4, 1999, at age 51. Every speaker at the conference, from academia and the national laboratory system, had received support through the program.

"It just blew my mind," says Hittinger, a Department of Energy Computational Science Graduate Fellowship recipient from 1996 through 2000 and now a computational scientist at LLNL. "Here you have all these top people in applied mathematics and scientific computing getting up and giving talks in memory of Fred and sharing memories of Fred." His reaction: "Wow, this guy is really something."

"I very quickly became aware of who he was and how important he was to researchers in the field," adds Hittinger, whose research focuses on methods for computational plasma physics.

So Hittinger understood the implications a few weeks later, when he was named one of two DOE CSGF alumni to receive the first Frederick A. Howes Scholar in Computational Science awards. Now in its tenth year, the award recognizes recent doctoral graduates of the DOE CSGF not just for their technical achievements, but also for outstanding leadership, integrity and character – qualities that brought Howes wide admiration.

The 13 Howes Scholars have gone on to careers in academia, at national laboratories and in private industry. At least one has founded a business. They're advancing the science in applied mathematics, chemistry, computational fluid dynamics, computer vision and artificial intelligence, geoscience, geography, drug design and other areas.

For each, the award affirmed their accomplishments, both technical and personal. "There's more to being a scientist, in some sense, than just the science," says Mala Radhakrishnan, a fellow from 2004 through 2007 and the 2008 Howes Scholar. Science also is working with others with integrity, says Radhakrishnan, now an assistant professor at Wellesley College, where she's researching computational design and analysis of drugs and biomolecules.

"To me, that's really important and it felt like that was validated" when she received the award, she adds.

For Mayya Tokman, a fellow from 1996 through 2000, joining Hittinger as one of two initial Howes Scholars "just gave me a boost of confidence" and "reassured me that what I'm doing is valued." She's now an assistant professor of applied mathematics at the University of California, Merced, where she studies methods for modeling complex, multiscale systems like astrophysical plasmas and biological cells.

Jaydeep Bardhan, a fellow from 2002 through 2006, was a postdoctoral researcher in Argonne National Laboratory's Mathematics and Computer Science Division when he was named a Howes Scholar for 2007. "People were coming down the hall, saying, 'Not only are we proud of you, but just so you know, Fred was one of the best guys around,'" says Bardhan, now an assistant professor in physiology and molecular biophysics at Rush University Medical Center in Chicago. "It became personal at that point."

HOWES SCHOLARS

2009 winner David Potere (left)
2008 winner Mala Radhakrishnan (left)
2007 winners Jaydeep Bardhan (left) and Kristen Grauman (right)
2006 winners Matthew Wolinsky (left) and Kevin Chu (right)
2005 winners Ryan Elliott (left) and Judith Hill (left)


2009


2008


2007


2006


2005

ACCOLADE'S NAMESAKE WAS FELLOWSHIP'S ADVOCATE

Frederick Howes was widely admired for his integrity, fairness, intelligence, humor and compassion, says Margaret Wright, then a researcher at Bell Laboratories and today a professor at the Courant Institute of Mathematical Sciences. His death was "a shattering blow" to friends and colleagues, and "the idea arose semi-spontaneously that we should do something concrete to honor his memory."

An informal committee soon decided that the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) was the most appropriate avenue for honoring Howes. His portfolio as manager of DOE's Applied Mathematical Sciences Program included the fellowship, which supports doctoral students who train in applied mathematics, computer science and an application discipline like biology, physics, engineering or materials science.

"Fred was a great champion of the CSGF, even when it was threatened" with budget cuts, Wright says, and he deserves credit for much of its early success.

The organizers wrote to those who had known Howes, Wright says, asking for contributions to the newly created Frederick A. Howes Scholar in Computational Science award. Those donations, plus a generous sum from Howes' family, built the foundation for an endowment. Others have since contributed as well.

DOE CSGF recipients who have completed or plan to complete requirements for their doctoral degree in a calendar year, both with fellowship support or after receiving support for the maximum number of years, are eligible for that year's Howes award.

Each fall the Krell Institute, which manages the program for the DOE, solicits nominations from department chairs, advisors and fellowship coordinators at universities qualified fellows attended. Nominations must include the names of at least two people who are familiar with the candidate's accomplishments.

Krell contacts the references to seek endorsements, and completed nominations — including the nomination letter — are sent to a review committee drawn from the national laboratory, academic and DOE CSGF alumni communities. One or two scholars are chosen to receive a cash award and an engraved crystal memento at the annual DOE CSGF conference in Washington, D.C.

It became even more personal when Howes' widow, Mary Hall, and son, Michael, made a rare appearance at the fellows' conference to participate in the presentation to Bardhan and Kristen Grauman, a fellow from 2001 through 2005 and now an assistant professor of computer science at the University of Texas at Austin. "It definitely makes you think that, 'All right, you have some living up to do,'" Bardhan says. Grauman, whose research focuses on computer vision and machine learning, says the honor "was completely unexpected. It meant a lot and it was a special occasion for me to come to the meeting."

At the conference, Howes Scholars also deliver presentations describing their research. For many recipients, the talk marks a transition from graduate school to careers in the field. It also could be their last opportunity to describe their research to an audience with widely varying interests.

"Science has become extremely specialized and people sit in a corner and work on their problems," Tokman says, but because fellows work in a range of application areas, conference speakers must make their research understandable to a cross-section of scientists. She says that made her 2001 talk both challenging and enjoyable.

"You have a room full of smart people … and you have the opportunity to describe what you do," says Tokman, whose lecture on modeling astrophysical plasmas included a "Star Trek" reference.

Bardhan, whose research focuses on simulation of large biological molecules, says he felt some pressure to present a first-class Howes Scholar lecture. The talks he'd heard from previous recipients — some of them good friends — were all top-notch and highly detailed.

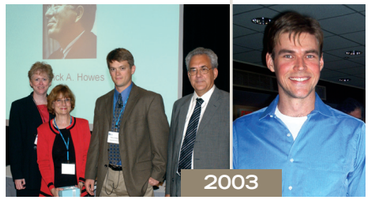
In the end, Bardhan says, his talk not only described his research, but also addressed the responsibilities fellows have when they "leave the cradle" and move into the field.

"We're in an environment where people don't always understand computational science very well or don't always know what high-performance computing can do," Bardhan says. It's CSGF graduates' job to enlarge the community, he adds.

Many Howes Scholars see the award as a commission to do just that. At Wellesley, "It's especially important … for students to see professors being recognized for research," Radhakrishnan says. Her award demonstrates that even a smaller institution can contribute to science, that professors strive to excel at both teaching and research and that women can thrive in technical fields. "That's a huge thing," Radhakrishnan adds.

Hittinger believes the award — and the DOE CSGF itself — have gained luster over the years as alumni have moved into top research and teaching posts, and that they're only going to become more prestigious. While that's boosted his career, Hittinger says the expectations accompanying the award may have had a greater impact.

"Maybe it's just the way I interpret it, but when you're given an award like the Howes Scholar, it's not just in recognition of what you've accomplished but also of your potential," Hittinger adds. "You have something you need to live up to."



2004 winner Collin Wick (right)
2003 winners Oliver Fringer (third from left) and Jon Wilkening (blue shirt)
2001 winners Mayya Tokman (second from left) and Jeffrey Hittinger (second from right)

2010 fellows directory GRADUATING CLASS

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Deterministic Transport Theory
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Iterative Methods for Linear Systems, Parallel Computing, Software for Scientific Computing
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Current Status: Staff Scientist, Los Alamos National Laboratory

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

Jimena Davis
North Carolina State University
Uncertainty Quantification, PBPK Modeling, Risk Assessment
Fellowship Years: 2004-2008
Current Status: Postdoctoral Fellow, US Environmental Protection Agency, Research Triangle Park, NC

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

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

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

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

Jeffrey Drocco
Princeton University
Biophysics and Computation
Fellowship Years: 2004-2008
Current Status: Graduate Student, Princeton Physics Tank Lab

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

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

Mary Dunlop
California Institute of Technology
Bioengineering, Synthetic Biology, Biofuels, Dynamical Systems
Fellowship Years: 2002-2006
Current Status: Postdoctoral Scholar, Joint BioEnergy Institute

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

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

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

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

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

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

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

Matthew Farthing
University of North Carolina
Flow and Transport Phenonmena in Porous Media
Fellowship Years: 1997-2001
Current Status: Research Hydraulic Engineer, USACE ERDC Coastal and Hydraulics Laboratory

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Ahna Girshick
University of California, Berkeley
Visual Perception (Computational Modeling and Psychophysics)
Fellowship Years: 2001-2005
Current Status: Researcher, New York University

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

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

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

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

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

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

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

Boyce Griffith
New York University
Computational Methods for Problems in Physiology
Fellowship Years: 2000-2004
Current Status: Medtronic/American Heart Association Postdoctoral Fellow, Courant Institute, New York University

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

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

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

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

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

Jeff Hammond
University of Chicago
Computational Chemistry on Supercomputers, Asynchronous Programming Models
Fellowship Years: 2005-2009
Current Status: Director's Postdoctoral Fellow, Argonne Leadership Computing Facility

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

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

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

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

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

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

Asegun Henry
Massachusetts Institute of Technology
Renewable Energy, Atomistic Level Heat Transfer, First Principles Electronic Structure Calculations
Fellowship Years: 2005-2009
Current Status: Postdoctoral Researcher, Oak Ridge National Laboratory

Judith Hill
Carnegie Mellon University
Computational Fluid Dynamics, PDE-Constrained optimization
Fellowship Years: 1999-2003
Current Status: Computational Mathematics, Oak Ridge National Laboratory

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

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

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

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

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

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

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

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

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

Amber Jackson
University of North Carolina
Applied Mathematics
Fellowship Years: 2004-2008

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

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

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

Peter Kekenes-Huskey
California Institute of Technology
Computational Chemistry and Biology
Fellowship Years: 2004-2007

Jeremy Kepner
Princeton University
Computational Cosmology
Fellowship Years: 1993-1996
Current Status: Senior Technical Staff, MIT Lincoln Lab

David Ketcheson
University of Washington
Applied Mathematics
Fellowship Years: 2006-2009
Current Status: Assistant Professor, KAUST

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

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

Bonnie Kirkpatrick
University of California, Berkeley
Computer Science
Fellowship Years: 2004-2008

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

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

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

Yury Krongauz
Northwestern University
Theoretical and Applied Mechanics
Fellowship Years: 1993-1996
Current Status: BlackRock (financial institution), New York City

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

Miler Lee
University of Pennsylvania
Computational Biology
Fellowship Years: 2005-2009
Current Status: Postdoctoral Researcher, University of Pennsylvania

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

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

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

Jeremy Lewi
Georgia Institute of Technology
Neuroengineering
Fellowship Years: 2005-2009

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

Lars Liden
Boston University
Biology
Fellowship Years: 1994-1998
Current Status: Chief Technical Officer, TeachTown, LLC; Software Technology Manager, University of Washington

Alex Lindblad
University of Washington
Explicit Transient Dynamic Finite Element Software Development
Fellowship Years: 2002-2006
Current Status: Senior Member of Technical Staff, Sandia National Laboratories – California

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

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

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

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

Marcus Martin
University of Minnesota
Monte Carlo Molecular Simulation, Primarily Focused on Algorithm Development
Fellowship Years: 1997-1999
Current Status: Director, Useful Bias Incorporated

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

Randall McDermott
University of Utah
Numerical Methods for Large-Eddy Simulation of Turbulent Reacting Flows
Fellowship Years: 2001-2005
Current Status: NRC Postdoctoral Researcher, NIST, Gaithersburg, MD

Matthew McGrath
University of Minnesota
Monte Carlo Simulations of Nucleation Phenomena
Fellowship Years: 2004-2007
Current Status: National Science Foundation International Research Fellow, Helsinki, Finland

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

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

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

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

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

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

Brian Moore
North Carolina State University
Computational Simulation of Nuclear & Thermal-Hydraulic Processes in Boiling Water Nuclear Reactors
Fellowship Years: 1992-1995
Current Status: Manager, Nuclear & Thermal-Hydraulic Methods, Global Nuclear Fuel

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

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

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

Michael Mysinger
Stanford University
Chemical Engineering and Quantum Chemistry
Fellowship Years: 1996-2000
Current Status: Arqule, Inc.

Heather Netzloff
Iowa State University
Quantum/Theoretical/Computational Chemistry
Fellowship Years: 2000-2004

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

Pauline Ng
University of Washington
Computational Biology
Fellowship Years: 2000-2002
Current Status: Informatics Scientist I, Illumina

Diem-Phuong Nguyen
University of Utah
CFD 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 Biology
Fellowship Years: 2006-2009

Joyce Noah
Stanford University
Theoretical Chemistry
Fellowship Years: 2001-2003
Current Status: Graduate Student, Stanford University

Peter Norgaard
Princeton University
Computational Plasma Dynamics
Fellowship Years: 2005-2009

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

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

Christopher Oehmen
University of Memphis/University of Tennessee, 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

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

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

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

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

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

Christina Payne
Vanderbilt University
Molecular Dynamics Simulations
Fellowship Years: 2003-2007
Current Status: Process Engineer, URS Washington Division

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

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 Years: 1997

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

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

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

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

Clifton Richardson
Cornell University
Physics
Fellowship Years: 1991-1995

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

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

Courtney Roby
University of Colorado
History of Science in the Ancient World
Fellowship Years: 2002-2003
Current Status: Graduate Student, Stanford University

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

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

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

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

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

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

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

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

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

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

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

Amoolya Singh
University of California, Berkeley
Dynamics and Evolution of Stress Response Networks
Fellowship Years: 2002-2006
Current Status: Computational and Life Sciences Postdoctoral Fellow, Emory University

Melinda Sirman
University of Texas
Engineering Mechanics
Fellowship Years: 1994-1996

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

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

Scott Stanley
University of California, San Diego
Fluid Mechanics, Turbulence Modelling, Data Handling for Large Datasets, Databases, Search Engines
Fellowship Years: 1994
Current Status: Hewlett-Packard

Samuel Stechmann
New York University
Applied Math, Atmospheric Science
Fellowship Years: 2003-2007
Current Status: Postdoctoral Researcher, University of California, Los Angeles

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

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

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

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

Brian Taylor
University of Illinois at Urbana-Champaign
Engineering Mechanics
Fellowship Years: 2003-2007

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, 3D Electron Microscopy
Fellowship Years: 2003-2007
Current Status: Finishing Ph.D.

Mario Trujillo
University of Illinois at Urbana-Champaign
Two-Phase Flow, Computational Fluid Mechanics, and Atomization Phenomena
Fellowship Years: 1997-2000
Current Status: Penn State University

Obioma Uche
Princeton University
Molecular Simulation, Statistical Mechanics
Fellowship Years: 2002-2006
Current Status: Postdoctoral Fellow, Sandia National Laboratories – California

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

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

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

Joshua Waterfall
Cornell University
Molecular Biology
Fellowship Years: 2002-2006
Current Status: Postdoctoral Researcher, Cornell University

Philip Weeber
University of North Carolina
Interest Rate Derivative Consulting
Fellowship Years: 1994-1996
Current Status: 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, and Nonlinear Optimal Control
Fellowship Years: 1991-1995
Current Status: Senior Engineer, Outer Planets Mission Design Group, NASA Jet Propulsion Laboratory, Pasadena, CA

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: Director's Postdoctoral Fellow, Mathematics & Computer Science Division, Argonne National Laboratory

Jon Wilkening
University of California, Berkeley
Numerical Analysis, Computational Physics, PDE, 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
Parallel and Combinatorial Scientific Computing
Fellowship Years: 2003-2007
Current Status: Postdoctoral Researcher, Sandia National Laboratories – New Mexico

Matthew Wolinsky
Duke University
Computational Geoscience
Fellowship Years: 2001-2005
Current Status: Research Scientist, Shell International Exploration and Production

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

Brandon Wood
Massachusetts Institute of Technology
Computational Materials Science
Fellowship Years: 2003-2007
Current Status: NSF IRPF Postdoctoral fellow, JNCASR, Bangalore, India

Lee Worden
Princeton University
Applied Mathematics
Fellowship Years: 1998-2002
Current Status: S. V. Ciriacy-Wantrup Postdoctoral Fellow, Environmental Studies, Policy and Management, University of California, Berkeley

Michael Wu
University of California, Berkeley
Social Analytics, Graph & Social Network Analysis, Predictive Modeling, High Dim 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: Research Scientist, Ohio Supercomputer Center

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

Etay Ziv
Columbia University
Computational Biology
Fellowship Years: 2004-2008

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

John ZuHone
University of Chicago
Astrophysics
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