THE DOE CSGF ANNUAL

DEXIS

2015

DEPARTMENT OF ENERGY COMPUTATIONAL SCIENCE GRADUATE FELLOWSHIP

BRIGHT IDEA

Eric Isaacs probes how metal nanoparticles supercharge sunlight's water-splitting feat

PAGE 5

THE DOE CSGF ANNUAL

DEIXIS

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

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

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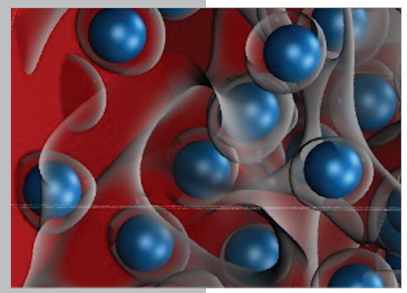

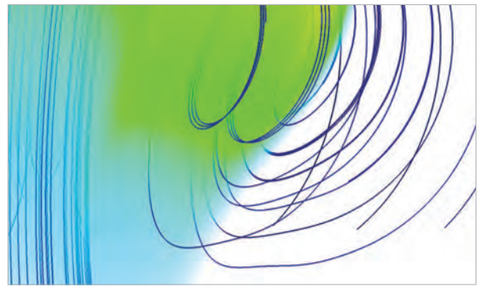

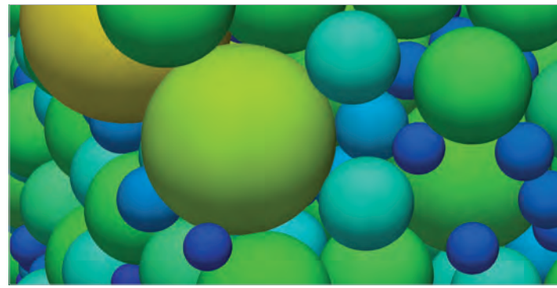

SUMMER APPLICATION

FELLOWS USE AND LEARN SKILLS ON PRACTICUMS

THE PRACTICUM is a highlight of the Department of Energy Computational Science Graduate Fellowship (DOE CSGF). For 12 weeks, fellows set aside their doctoral research and work alongside scientists at DOE national laboratories.

As the word denotes, the emphasis is on practice: Fellows apply what they've learned to problems of national importance.

For example, Eric Isaacs left Columbia University for Brookhaven National Laboratory on New York's Long Island, where he helped decipher a photocatalytic effect that splits water molecules. The project was only tangential to his doctoral inquiries into potential new battery materials.

At the University of California, Irvine, Aurora Pribram-Jones usually relied on models to refine methods to calculate materials' electronic structures. At Sandia National Laboratories in New Mexico, however, she tackled real-world shock physics computations.

At Stanford University, Aaron Sisto researched the fundamental details behind light-harvesting bacteria. But at Lawrence Livermore National Laboratory in California, he learned tools to mathematically identify the most influential properties for making three-dimensionally printed metal parts.

All three fellows can attest to the impact of the practicum.

As the word denotes, the emphasis is on practice: Fellows apply what they've learned to problems of national importance.

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The Department of Energy Computational Science Graduate Fellowship supports the nation's brightest science and engineering students, allowing them to concentrate on learning and research. The work of more than 325 DOE CSGF alumni has helped the United States remain competitive in a global economy.

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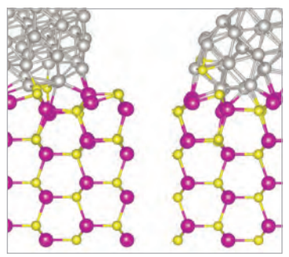


Image courtesy of Shangmin Xiong

SHINING A LIGHT ON WATER-SPLITTING REACTIONS

ERIC ISAACS
Columbia University
Brookhaven National Laboratory

AS A YOUTH, ERIC ISAACS MOVED from the Midwest to the West Coast. He went from there to the East Coast for his doctoral studies. But he traveled less than 70 miles for his 2013 practicum.

Isaacs, a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient, studies applied physics at Columbia University in New York. His practicum was just a couple hours away (in light traffic), at Long Island's Brookhaven National Laboratory.

For Isaacs, an intellectual bond was more important than physical proximity. "I was interested in forming connections to researchers at Brookhaven and in knowing what's going on there," he says, since it's packed with experts and high-performance computers.

As a youth, Isaacs lived in a Cleveland suburb, but attended high school near Los Angeles after his father, a surgeon, relocated the family. At the University of California, Berkeley, Isaacs first majored in chemistry, but was frustrated by how little his introductory courses discussed chemical principles' underlying mechanisms. He switched to physics because "it seemed to be the most fundamental way of looking at nature – going down to the lowest level."

This first-principles, or *ab initio*, approach is key to Isaacs' doctoral research under Chris Marianetti, associate professor of materials science and applied physics and applied mathematics. They develop quantum mechanical models to track how electrons behave in complicated materials, hoping to find compounds that make batteries hold more electricity while absorbing and releasing it efficiently.

"We're using computer simulations to predict, rather than measure directly, properties of materials, particularly properties relevant to actual things you'd want to do with these materials," such as store energy, Isaacs says.

Isaacs' summer project with computational scientist Yan Li was more about explaining materials' properties than predicting them. It arose from experiments at Stony Brook University in New York State, where researchers study cadmium sulfide, a semiconductor. When exposed to sunlight, it acts as a weak photocatalyst for hydrogen production from

STRETCHING TO A SURPRISING RESEARCH RESULT

The project Eric Isaacs took as he joined Chris Marianetti's materials science and engineering group proved more interesting than a mere exercise to learn new techniques.

The subject was monolayer materials: sheets between one and a few atoms thick that are remarkably strong and have unusual properties. In a previous study, Marianetti's group found that graphene, a single layer of carbon atoms, underwent a surprising transition as it broke under stress. He suggested Isaacs see what happens to other monolayers under similar conditions.

Using Brookhaven National Laboratory supercomputers, Isaacs modeled graphene, boron nitride, molybdenum disulfide and graphane (graphene in which each carbon atom bonds with a hydrogen atom). Many such monolayers are built of six-atom backbones linked like a hexagon. The simulations stretched the sheets equally in all directions.

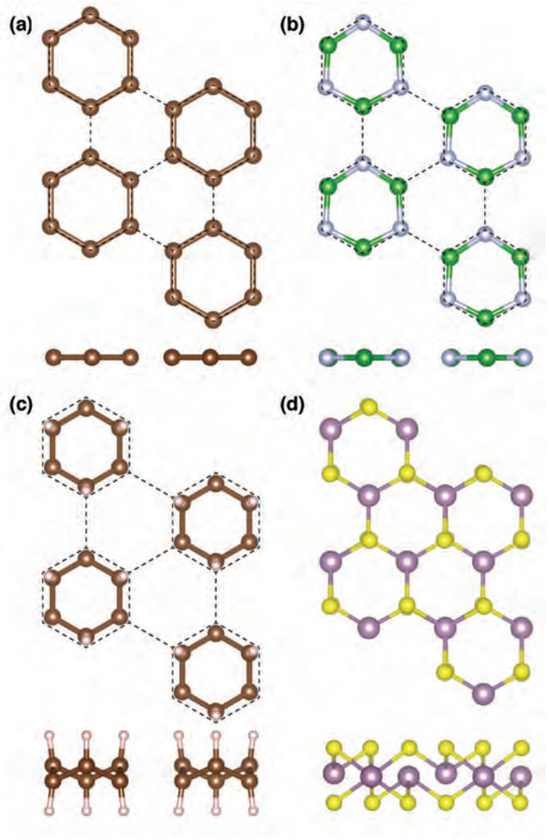
In monolayer materials, as in all substances, atoms rapidly vibrate in place. In most cases, stretching leads to elastic instability, in which atomic bonds continuously break and the material separates uniformly.

Isaacs' models indicate that monolayer materials' vibrational modes change under stress. "There's a subtle instability that happens" instead of elastic instability, he says. "The material will not just start vibrating in that mode and return to equilibrium, but will keep going," essentially transforming into a new structure. In this "soft mode" the molecules tend to separate into isolated hexagons.

In an elastic instability model, the new structure will break by that point. "In these calculations, we're not seeing the actual breaking process, but we're predicting when it would happen and what the mechanism is." It turns out this change from the beginning vibrational mode into another unstable structure limits the materials' strength.

This instability was unexpected, but it was more surprising that all the materials were susceptible despite their different electronic properties. Isaacs "generalized this for most of the monolayer materials," Marianetti says. "What he showed, which was not obvious, is that most of them shared a very similar, if not identical, instability. It was beautiful work."

The results could help researchers better predict the strain a material can take and find ways to delay or overcome this soft mode to strengthen substances.



Projections from the top and side of distorted structures for (a) graphene, (b) boron nitride, (c) graphane and (d) molybdenum disulfide each strained equally in all directions. The carbon, boron, nitrogen, hydrogen, molybdenum and sulfur atoms are represented as brown, green, silver, white, purple and yellow spheres, respectively. Dashed lines indicate the undistorted strained lattice. In graphene, boron nitride and graphane the backbone distorts toward isolated six-atom rings, while molybdenum disulfide undergoes a distinct distortion toward trigonal pyramidal coordination. *Reprinted with permission from E.B. Isaacs and C.A. Marianetti,* Phys. Rev. B *89, 184111 (2014).*

'We're really focused on why it works and what's going on at the atomic level.'

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water. The team found sprinkling a slab of the material with nanoparticles, each made of a few dozen gold atoms at most, increases hydrogen generation by as much as 35 times. They also found platinum, a common catalyst, had a similar effect.

The process could help make hydrogen a clean, plentiful energy source, but it's puzzling. "Gold is an inert noble metal. You think it's not going to be that chemically active," Isaacs says. Exactly why it and platinum (another noble metal) supercharge the reaction is "a big scientific question."

Li, now an editor for the journal *Physical Review B*, and her team wanted to model interactions between the cadmium sulfide and the nanoparticles. They wanted to calculate how atoms at the interface transfer negative or positive charges and how electron energy levels in the nanoparticles align with those in the substrate.

"Part of the reason we were studying this is for fundamental reasons: to know how we can use these catalysts and nanotechnology to improve this reaction," Isaacs says. "We're really focused on why it works and what's going on at the atomic level."

To get there, Li uses density functional theory (DFT), an *ab initio* technique that accounts for quantum mechanical conditions in which electrons behave as both particles and waves.

AGAINST THE GRAIN

First the models needed to describe how atoms are arranged in the crystalline cadmium sulfide surface. Different arrangements lead to different surface qualities, like structure and charge polarity, that affect interactions with the nanoparticles. It's a bit like how wood cut against the grain differs from wood cut with the grain. Isaacs and Li used the Vienna Ab initio Simulation Package, a popular electronic structure code, to model these configurations and compute their properties.

"A crystal has different facets," Li says, and researchers must know which facet is at the surface before simulating it. Experimental data gave few clues as to the correct one "so we had to try ourselves."

Using the Python language, Isaacs wrote a script to cut the simulated cadmium sulfide surface along a crystal orientation. "I didn't teach him anything," Li says. Isaacs studied a software tutorial, then "generated a surface, all by himself. That was very impressive."

Isaacs investigated how rearranging atoms near the surface affects the substrate properties. He researched surfaces with either polar (having nonzero dipole moment – separated positive and negative charges) or nonpolar orientations and probed their electronic properties. For polar cadmium sulfide surfaces, Isaacs examined cases in which the surface terminated with cadmium atoms versus sulfur atoms.

The polar surface configuration the researchers tried in an early simulation produced answers that matched poorly with research data. Before the practicum ended, they deduced that a nonpolar molecular orientation works better.

Because it's arduous to exactly calculate interactions at the cadmium sulfide surface, the team also needed a simplified representation of the noble metal nanoparticles. Isaacs researched the scientific literature to devise one. "It's pretty challenging, if you're not an experimentalist, to make some educated guess on the best model," he adds. "We worked with our experimentalist friends to help out, but there was a lot of digging."

Computations ran at the National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory and on a cluster at Brookhaven's Center for Functional Nanomaterials.

Isaacs is a coauthor on a paper, published in the *Journal of Physical Chemistry C*, reporting the simulations of platinum nanoparticles on a nonpolar surface. The first author, Stony Brook graduate student Shangmin Xiong, did much of the work, Li says, but Isaacs "really helped to kick-start the project." He knew the theory behind the models and already was familiar with the computer codes to run them. "It only took a couple days to let him start doing some calculations," Li says. "This was definitely a happy surprise."

Results indicate that nanoparticle size greatly influences the water-splitting effect, Li says, but it's unclear which works best with the surface to promote the reaction. Simulations can help unravel this, but they'll require more detailed – and demanding – approaches, she adds.

Isaacs presented a poster on the practicum work at a Brookhaven Young Researcher Symposium in November 2013. Marianetti says the experience "widened (Isaacs') view by pushing him into an area of problems that he wouldn't have seen in my research group."

MAKING A TRANSITION

That perspective could help as Isaacs investigates materials containing transition metals: elements with partially filled electron shells, allowing them to easily receive and donate electrons – a key battery cathode material property.

Most transition metal compounds in cathodes are oxides, with the metal coupled to oxygen atoms. Many already are in devices like cellphones. But numerous transition metal oxides are
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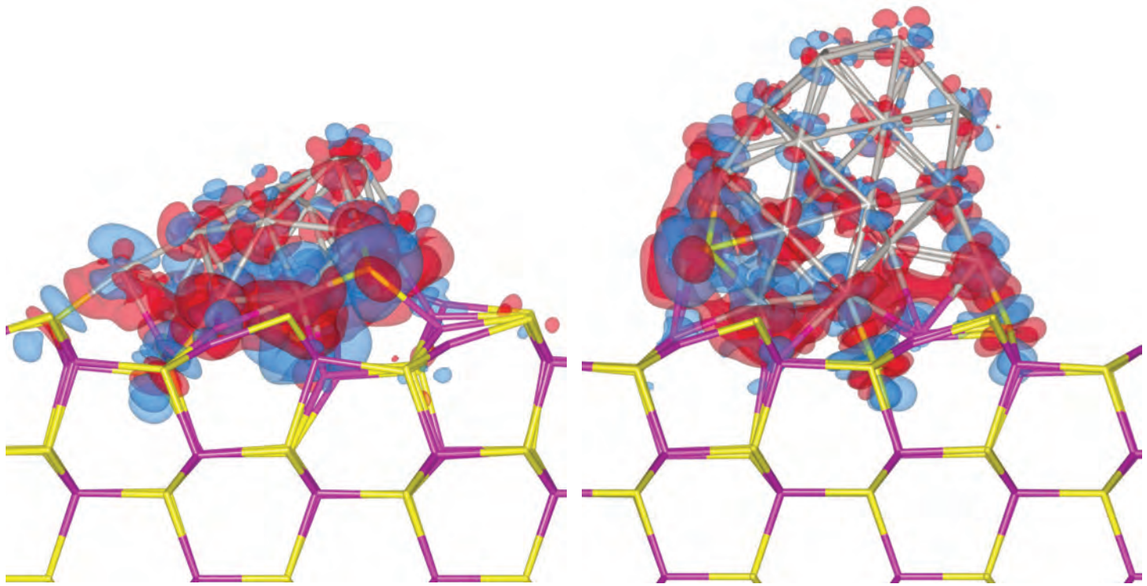

Electron density difference isosurfaces after the adsorption of a 19-atom platinum cluster (left) and a 38-atom platinum cluster (right) on a cadmium sulfide surface. Red and blue denote electron gain and loss, respectively. *Image courtesy of Shangmin Xiong, from "Adsorption characteristics and size/shape dependence of Pt clusters on CdS surface," S. Xiong, E. Isaacs and Y. Li, J. Phys. Chem. C, 2015, 119 (9), PP 4834-4842.*

strongly correlated materials – "notoriously difficult to understand" substances, Isaacs says. "To go beyond the current technology and even just to better understand how it works, we need to improve our descriptions of strongly correlated materials and to predict properties of new ones."

DFT maps the many-body problem, in which every electron interacts with every other electron, onto an easier, non-interacting electron problem. But in strongly correlated materials, some electrons interact intimately. "Because of that, it's very difficult, or in some sense impossible in practice, to model the material at a level that considers just single electrons," as DFT does, Isaacs says.

Take, for example, lithium iron phosphate, a promising battery material Isaacs studies. DFT, Marianetti says, "claims you should be able to diffuse lithium in and out and it should mix" as the battery charges. Experiments show just the opposite: It separates into phases of iron phosphate and lithium iron phosphate, limiting how fast the battery can charge and discharge.

To understand this and other strongly correlated materials, Marianetti's group combines DFT with dynamical mean field theory (DMFT). It calculates electron interactions more explicitly, but can't cope with a huge number. Instead, it calculates strongly correlated interactions while DFT accounts for the rest.

Marianetti says his group has worked on combining DMFT and DFT, but "Eric is pushing forward toward actually applying this to battery materials, which would be sort of a massive leap."

It's a perfect subject, Isaacs adds: "We're looking at questions of basic science, but we're also looking at a technologically relevant material in hopes this can make an impact."

In his off hours, Isaacs sometimes makes a different kind of impact: punching an opponent in the boxing ring. "It's good exercise," he says, and "very helpful to reset after so much of reading papers and coding."

Isaacs aims to knock out his doctorate sometime in 2016. Regardless of where he works, he wants to connect his research with everyday products that improve life.

After all, "the battery in the cellphone I'm using right now was only an idea in a lab not long ago."

'Big science is very different from what I get to experience every day.'

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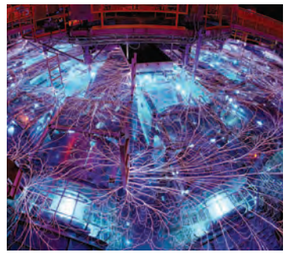

Credit: Sandia National Laboratories

PUTTING THEORY INTO PRACTICE, UNDER PRESSURE

AURORA PRIBRAM-JONES
University of California, Irvine
Sandia National Laboratories, New Mexico

AURORA PRIBRAM-JONES DEALS in the intangible in her theoretical chemistry doctoral research at the University of California, Irvine. She tinkers with algorithms' innards, using desktop computers to test new methods on model problems. "Big science is very different from what I get to experience every day," she says.

Pribram-Jones got a regular dose of big science on her 2013 practicum at Sandia National Laboratories in New Mexico. The Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient used high-performance computing (HPC) systems to examine real materials. She worked with engineers and physicists who design and run high energy density physics experiments. Many of the tests take place on the Z Pulsed Power Facility, or Z machine, a warehouse-sized device that delivers tremendous energy to tiny targets. The pulses subject materials to unearthly pressures and temperatures.

Pribram-Jones was based nearby. "It's so cool," she exclaims. "You know it's running every day, because you get the shudder in your office when they send it down line."

The practicum expanded Pribram-Jones' research skills, which focus on refining techniques to understand matter's fundamental properties under extreme conditions. Her work can edge us toward greater knowledge of the universe and potential new energy sources.

What Pribram-Jones learned in her journey to graduate school, however, is as important as her classroom education. Her talents would have mattered little without determination and help from understanding educators.

Pribram-Jones grew up in East Palo Alto, California, next door to Palo Alto, the home of Stanford University. Both her parents fought drug addiction and her father's health failed, putting him out of work as a fire protection system installer. After that, "we got pretty poor pretty quickly," she says. Her mother, a teacher, struggled to hold the family (including Pribram-Jones' younger brother) together while fighting her own addiction and mental illness.

Despite their problems, "my parents were really amazing people," Pribram-Jones says. Books were plentiful and her mother, a neuroscientist's daughter, raised her children to think scientifically, even when making sandwiches. If someone put the peanut butter lid on the counter face down, her mother would warn, "You're going to contaminate your sample."

Pribram-Jones never completed high school, but passed proficiency tests that allowed her to enroll as a music major at Foothill College, a community college. At 15, Pribram-Jones moved to Southern California for a year in a search for stability. Her father died a year after she returned to East Palo Alto. She tutored students in bassoon, math and reading and worked other jobs to help support her family.
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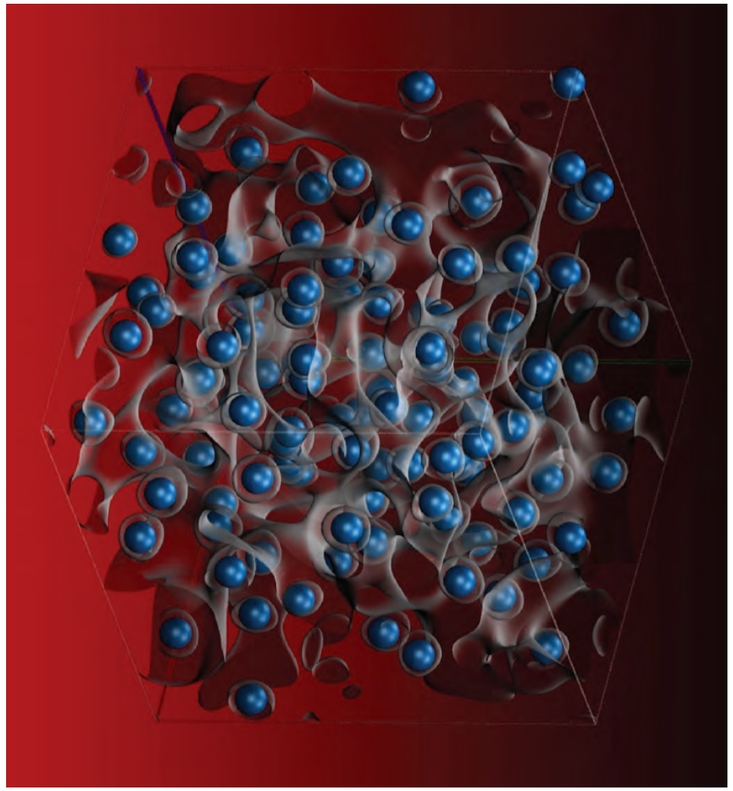

This snapshot from a molecular dynamics simulation shows the hot disordered state of aluminum as the material releases toward ambient pressure following a high-pressure shock, with an added isosurface (three-dimensional representation) of electron charge density. It shows some of the electrons localized near ions while others fill a continuum between the atoms. Aurora Pribram-Jones's thesis research has helped develop a deeper understanding of the precise electron density distribution under these warm dense matter conditions. *Image courtesy of Michael Desjarlais, Sandia National Laboratories.*

A few years later, Pribram-Jones was managing a Palo Alto bookstore. She often stayed after closing and fell asleep while reading books from the technical section. When she returned to Foothill in 2003, Pribram-Jones had learned enough to test out of chemistry and math classes. She earned simultaneous associate's degrees in chemistry, math and biology.

A NEW OBSTACLE

Pribram-Jones transferred to Harvey Mudd College, a small California school known for its emphasis on engineering, science and math, and did well in her first year. But one morning she awoke to find her left arm paralyzed. Doctors found the cause – ruptured discs in her neck had impinged on a nerve – but also discovered a benign tumor in her collarbone. Pribram-Jones took a year off to recover and deal with a mountain of medical bills – but still sat in on classes.

"I had worked very hard to get there, so I felt I had really failed," she says. Understanding professors gave her jobs in a chemical stock room and assisting with labs, and she returned to graduate in chemistry. "It was definitely very hard and I'm lucky I had advocates on the faculty." That experience pushes her to help others as a teacher and mentor, a mission she plans to continue after earning her doctorate this year.

Pribram-Jones chose theoretical chemistry for graduate school because it connects two favorite subjects – chemistry and math – but also because she was unsure whether she could handle theory. "I tend to choose the path that I find scariest," she says, because she learns new things.

Her difficult circumstances have given Pribram-Jones an unusual intellectual maturity, says Kieron Burke, her doctoral advisor. "I think it comes from being exposed to many different environments and dealing with all sorts of situations. … What comes up in academia is child's play relative to some of the things" Pribram-Jones has faced. What's more, he says she grasps the logical abstraction his research requires in a way few students can. "There's only a dozen or so people in the world who can really think that way and she will become one of them if she keeps at it."

Burke and Pribram-Jones focus on density functional theory (DFT), a technique to calculate electron interactions in molecules. It's an *ab initio* method: Preset conditions or experimental data don't inform the simulations. The method applies fundamental rules from the strange world of quantum mechanics, in which electrons can be both particles and waves.

DFT is accurate but consumes less computer resources than other quantum chemistry techniques, making it computational chemists' go-to method. It's used on complex problems in energy, physics and chemistry.

Rather than apply DFT to real materials, however, Pribram-Jones probes its mechanisms. "I work on things that elucidate how the actual theory itself works," using "math tools and physics tools to look at fundamental problems so we can use insights from those to crack open more complicated problems." Instead of studying real materials, they're "like thought experiments. They allow us to start peeling the onion and get to more interesting, fundamental pieces of information."

The phenomenon Pribram-Jones wants to help others understand with her DFT ideas is warm dense matter (WDM), a high-temperature, high-density state between plasma and solid but with properties of both. WDM is found in explosions and deep inside planets, especially gas giants like Saturn. Inertial confinement fusion (ICF) experiments, like those at the Department of Energy's National Ignition Facility, also create WDM in tiny capsules of frozen hydrogen.

"It's either very expensive or impossible to do experiments on matter in those conditions," Burke says, so mathematical methods to predict WDM properties are critical.

UNDER PRESSURE

WDM also is found in shocked materials – like those tested in the Z machine. Sandia Senior Scientist Michael Desjarlais, Pribram-Jones' practicum supervisor, builds *ab initio* models that often emulate or predict Z experiments. Desjarlais and his colleagues use DFT and other methods to calculate what happens when materials like diamond are subjected to extreme conditions, as in a terrific shock. The results go into complex codes simulating the interiors of giant planets, ICF experiments, and other phenomena.

At Sandia, Pribram-Jones first learned to use the Vienna Ab initio Simulation Program (VASP), a code combining DFT with molecular dynamics, a classical physics technique. She used it to compute two key properties for aluminum: the high-pressure Hugoniot and the release isentrope.

The Hugoniot is like a line on a graph. To find each point, researchers strike a material (aluminum in this case), usually starting at ambient temperature and pressure, with a powerful shock. Researchers can add points to the graph by performing successively stronger shock experiments. With each one, Desjarlais says, "I get a new end state (in the material) that is a slight increase in density and increase in pressure." Plotting those points yields the Hugoniot. "It's a way of encapsulating all the different responses of that ambient material to a variety of shock strengths."

The release isentrope comes after the shock passes. With nothing to confine the material, it expands isentropically – without heat entering or leaving. "The material doesn't go back to its initial state when you release it, because when you shocked it you dramatically increased its entropy," or thermodynamic disorder, Desjarlais says. For example, the material could be shocked into a plasma state that dissipates into the surrounding environment. The release isentrope is different for each Hugoniot point.

In the past, researchers used theoretical models to produce equation of state tables from which scientists could extract Hugoniot points and release isentropes, Desjarlais says. But for "high-fidelity work, like the work we do on the Z machine, those tables are often not accurate enough." For improvement, researchers turn to *ab initio* DFT calculations like the ones Pribram-Jones did on her practicum. "The Z machine is an amazing, amazing experimental tool," she says, but it's impossible to test materials under all the

'I tend to choose the path that I find scariest.'

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conditions important to science. It's crucial "to have calculations we can predict will work well at a certain temperature or pressure range."

Researchers use aluminum as a benchmark material to help deduce the properties of other materials in a shock experiment. Pribram-Jones' work will contribute data to a new standard for aluminum, Desjarlais says.

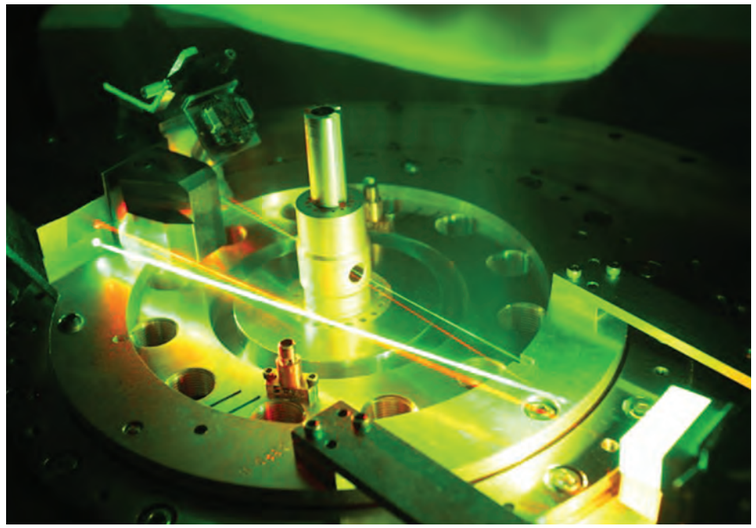
Another part of Pribram-Jones' project aimed to cut the computer time needed to calculate release isentropes. She compared the accuracy of a method Desjarlais developed with another that's simpler to compute but thermodynamically approximate.

Pribram-Jones ran VASP simulations using both methods and analyzed the results. Both techniques calculate isentrope points and use a Mathematica tool to determine where to do the next step, but the simpler technique uses fewer intermediate steps, Pribram-Jones says. She determined the simpler method was sufficiently accurate for most purposes, Desjarlais says, giving researchers the confidence to use it more freely.

Since leaving Sandia, Pribram-Jones has continued collaborating with Desjarlais to calculate the aluminum Hugoniot and isentrope values at even more extreme pressures and temperatures. She's also contributing to a paper on the research.

The practicum plunged Pribram-Jones deep into high-performance computing for the first time. Using Red Sky, Sandia's Sun Microsystems supercomputer, was "like learning to drive in a Ferrari," she says. "It was very, very different than the model calculations I do."

Burke says the experience made Pribram-Jones better at intuitively recognizing when an algorithm's results are illogical. The big benefit, however, was working with experts in vastly different subjects from her usual area. "You don't get that kind of thing without doing something like a practicum."

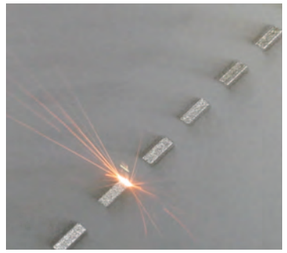


Lasers are used to align diagnostics and hardware prior to shooting on Sandia's Z machine. Computer models predict and emulate experiments on the giant pulsed-power device. *Credit: Sandia National Laboratories.*

CONDUCTING ENSEMBLES TO FERRET OUT FEATURES

AARON SISTO
Stanford University
Lawrence Livermore National Laboratory

More than 130 factors affect the final product's quality.



Credit: Lawrence Livermore National Laboratory

WHEN HE STARTED his 2013 Lawrence Livermore National Laboratory (LLNL) practicum, Aaron Sisto just wanted to learn data mining techniques.

Yet the project he completed may also help advance additive manufacturing – three-dimensional printing – and has led him to found his own company.

Sisto, a son of Chicago artists, is driven to find real-world applications for what he learns and discovers. He studied mechanical engineering at Purdue University because it focused on the practical aspects of design and creation. Later, Sisto says, he became interested in peripheral subjects that required a perspective outside his field. He switched to computational chemistry for his doctoral studies at Stanford University and earned a Department of Energy Computational Science Graduate Fellowship (DOE CSGF).

Sisto's quest for new perspectives also pushed him to work with Chandrika Kamath of LLNL's Center for Applied Scientific Computing and learn techniques for finding the key nuggets in mounds of information. He studied feature selection algorithms, mathematical methods to identify the most influential variables in a data set.

Kamath, an experienced data-mining researcher, and her colleagues provided Sisto a good test for his new skills: selective laser melting (SLM), in which a powerful beam fuses metal powder particles, layer by layer, into a solid object. It's a versatile but complex 3-D printing technology: More than 130 factors affect the final product's quality.

The LLNL team wanted to identify the combination of SLM parameters needed to create stainless steel parts with greater than 99 percent density. They could have printed dozens of tests, each with a different blend of parameter settings, to find the best mix, but that would consume huge amounts of time and money. They needed to limit the parameter space to only the most influential factors.

Kamath's role was to use simple simulations and experiments to quickly find the key process parameters for high-density parts. Other LLNL scientists had run a model to calculate the length, width and depth of the melt pool – the puddle formed when the laser hits the bed of powder particles. Each simulation combined four parameters: power, scan speed, beam size, and how much energy the material absorbs.

Centering the simulations on just four parameters still left a significant data problem, as each can have a range of settings, like 10 different scan speeds and seven power levels. Kamath wanted to answer the question of whether any of the four parameters had a greater effect on density than others.

That connected to Sisto's feature-selection work. "It just so happened we were working on this additive manufacturing problem and there were data from some of the simulations," Kamath says. "So it seemed like one could apply those techniques (Sisto) was implementing to this data set."

'You can turn light into any form of energy you want and direct it in any way that's useful.'

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Sisto first investigated feature-selection algorithms, which identify the most influential parameters or rank them by importance. There are numerous such methods, Kamath says, but the biases in each can suggest varying paths, similar to how opinion poll results can diverge.

CONDUCTING THE ENSEMBLE

"When you use any of these techniques, you have to be very careful because the outcome might be dependent on what data set you're working with," she says. "You never really apply these techniques blindly." Instead, researchers often use an ensemble of methods and average their conclusions to improve accuracy, like how averaging opinion polls can predict an election more accurately than any individual poll.

Sisto used the C++ programming language to build an ensemble of five feature-selection algorithms. Each evaluated the relative importance of the four factors used in the laser simulations – power, scan speed, beam size and absorptivity – and rated each for its effect on the melt pool. Each feature-selection algorithm ranked the parameters on a five-point scale from least important to most important.

Still, Sisto says, ranking "doesn't necessarily tell you that the highest rank is the most important and the lowest is completely unimportant. All that tells you is relative to each other, that's where they stand." To further refine feature selection, the program includes a fifth parameter: noise, or a measure of random data variation.

If certain features rank lower than this noise baseline, then Sisto could throw out those features, further reducing the parameter space. "We know anything ranked below random noise is absolutely unimportant," he says, much as candidates polling below a certain level can be regarded as having no impact on an election.

The results indicated that scan speed and laser power affected melt-pool width and depth the most, whereas power and the material's ability to absorb that power most affected length. Other factors generally ranked below the noise baseline.

With that information, Kamath and her fellow researchers geared experiments toward power and scan speed, using SLM to build one 10-mm square, 7-mm tall stainless steel pillar for each of 48 combinations of the two. The best densities resulted when the laser power was highest (400 watts), even when speed varied from 1,900 mm per second to 2,200 mm per second, said an *International Journal of Advanced Manufacturing Technology* paper Sisto coauthored with Kamath and Livermore scientists Bassem El-dasher, Gilbert Gallegos and Wayne King.

The results were consistent with the ensemble's predictions, Sisto says. "This analysis directed the search in two of these parameters. If there had been hundreds (of parameters), this would never have been possible."

Sisto worked to give the package, named redDRC (reduced dimensionality, regression and classification), a usable interface and to ensure it could handle a variety of problems and data sources. He still contributes to its development.

Sisto appreciated the practicum's introduction to data mining. "It was a great way to learn about it from Chandrika, who has years of experience. I think I got a neat perspective on the applied side." For her part, Kamath says she had hoped Sisto "would at least learn something about different techniques and appreciate the issues in applying them to real data. From that point of view, it was a successful practicum."

Sisto's doctoral advisor, Todd Martinez, says the experience sharpened Sisto's ideas about using computers, with machine-learning and data-mining tools, to design molecules. "That's really what drives him," he adds.

Those ideas also pushed Sisto to start QComponents, a company offering rapid design and prototyping of new molecular electronics. Such activities often are time-consuming and expensive for high-tech firms, he says. "The idea was to use skills I have in high-performance computing and in simulation and data mining and put those into an integrative framework" to help companies.

At Stanford, Sisto builds detailed computer models of excitation energy transfer: Electrons are boosted to higher energies by light or other sources and then interact with the environment to transport that electronic energy across multiple molecules.

A LIGHT CROP

It's key to light harvesting: how organisms convert photons into chemical energy. What Sisto and Martinez, the David Mulvane Ehrsam and Edward Curtis Franklin professor in chemistry and professor of photon science, learn could help scientists harness biological molecules for specific purposes or build their own.

Sisto's techniques capture the strange effects of quantum mechanics and work from first principles: starting without preset conditions or empirical data. Such *ab initio* calculations can track the complex interactions between electrons in atoms.

Sisto and Martinez concentrate on light-harvesting complex II, a structure found in photosynthetic bacteria. It's comprised of chromophores – molecules that capture light energy. The problem, Martinez says, is "excitation transfers from chromophore to chromophore, and each chromophore is typically between 50 and 200 atoms."

Modeling even a few dozen atoms from first principles requires powerful computers. Martinez says Sisto leapt the hurdle through a combination of physical insight and computing prowess. The insight: Although electron interactions are tightly coupled within each chromophore, coupling between chromophores is weak. "Rather than having all the electrons talking to each other at once, you can solve the problem in pieces," Martinez says, tracking interactions within a chromophore but "only talking very weakly to the remainder of the system."

Sisto says the algorithm runs on hybrid high-performance computers – ones using both standard processors (CPUs) and graphics processing units (GPUs), video game chip descendants now found in many of the world's fastest machines. The algorithm uses a parallel hierarchy: At the top level, individual chromophores are sent to computer nodes comprised of GPUs and CPUs for simultaneous calculation. Building on Martinez's earlier GPU research, processors in the hybrid nodes also work in parallel to compute the chromophore's complex electronic interactions at the lowest level.

"Then we patch the system back together in an extremely efficient way that gives you back all the information about this massive complex," Sisto says.

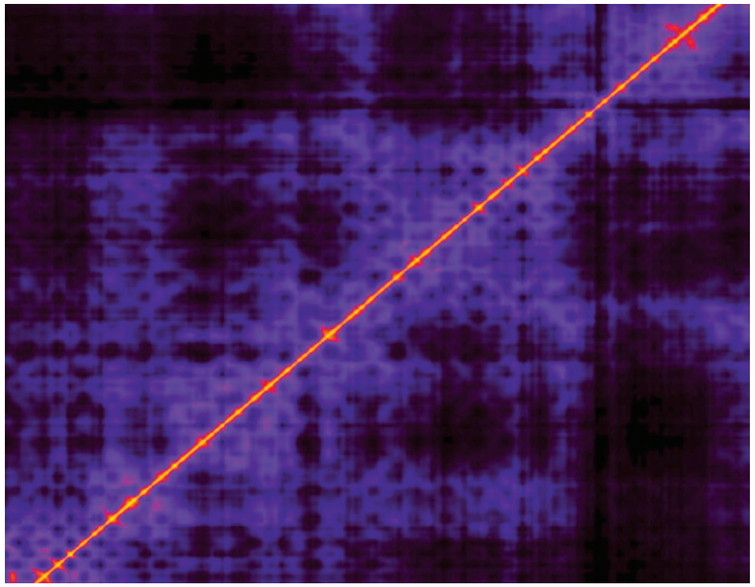
Joining chromophores to calculate a light-harvesting system's total energy isn't a new idea, Martinez says, but it usually was used to fit parameters so the model results matched observed phenomena. Sisto instead uses the chromophore model as an organizing framework for first-principles calculations, without fitting data. "The real genius of all this," Martinez says, is to take "ideas that were used as models where you would fit data, and turn that into a coarse-graining principle" for parceling out work.

As a result, Martinez says, the method can calculate excitation dynamics in molecules of at least 4,000 atoms. That could make it a candidate to run on an exascale computer capable of a million trillion (10^{18}) calculations per second, about a thousand times faster than today's best machines.

By helping scientists understand light absorption, Sisto says, his algorithms may one day lead them to tune the process in useful ways. "That will open up a range of possibilities, because you can turn light into any form of energy you want and direct it in any way that's useful."

For now, Sisto is considering how his methods can be applied more generally to make better decisions and reach milestones more efficiently – one of his goals for QComponents.

With "molecular design just on the cusp of being relevant to industry," Martinez says, the company may be how Sisto distinguishes himself. "He could make an impact there."



This visualization shows the similarity matrix that describes the relative distances between individual points in a data set used to test an ensemble feature-selection algorithm. Each point in the plot represents the similarity between two data points, with light-colored elements denoting high degrees of similarity and dark colors indicating low similarity. *Image courtesy of Aaron Sisto.*
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FROM ALUMNI TO LEADERS

Helping Users Get Science From Titan

Matthew Norman
Oak Ridge National Laboratory

WHEN MATTHEW NORMAN STARTED as a computational climate scientist at Oak Ridge National Laboratory in 2011, he thought he may be unqualified to work with Titan, one of the world's biggest, most powerful machines.

"I had my worries coming in that I wouldn't necessarily know what to do, but then I quickly realized that no one does until they get here," says Norman, a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient from 2008 to 2011. "Everyone has an idea of how you debug a code until you're doing it on the order of 10,000 nodes. It completely changes the way you need to approach it."

Four years later, Norman qualifies as something of an old hand as he helps adapt codes to run on Titan, a Cray XK7 at the Oak Ridge Leadership Computing Facility. Titan's architecture includes a combination of standard central processing units (CPUs) and graphics processing units (GPUs), video-game chip siblings that accelerate calculations. The mix makes it tricky for existing programs to run on Titan.

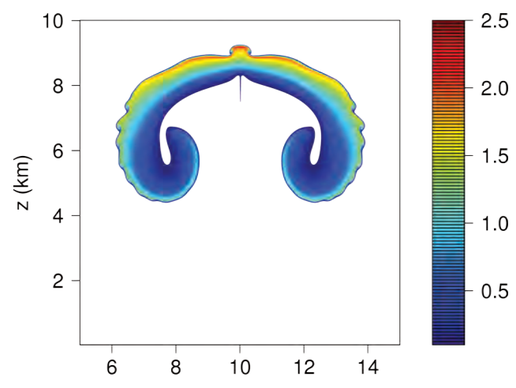
Norman's experience is tested as a liaison to researchers awarded computer time from the Department of Energy's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. It grants millions of computer processor hours on Titan and other DOE supercomputers to scientists from government, academia and industry. Norman and his colleagues are essentially embedded in research teams to help codes produce science on Titan.

OVERCOMING OBSTACLES

"I've worked on earthquake hazard codes and climate codes and even a quantum Monte Carlo code," Norman says. Each has its own obstacles to running on Titan – ones Norman tries to conquer by profiling the program to see where it expends resources, such as on communication or system overhead, or by reproducing and solving problems. "It's making sure (researchers) can get science out of the code as efficiently as possible."

In a similar vein, Norman oversaw porting the Community Atmosphere Model-Spectral Element (CAM-SE) to Titan. CAM-SE is part of the larger Community Climate System Model in DOE's Accelerated Climate Modeling for Energy program. The Spectral Element Method (SEM) variant requires less parallel communication than other CAM versions as the processors calculate physical changes in each part of the atmosphere. That means CAM-SE scales better and can run on more processors than other versions. Porting CAM-SE to run on GPUs produced a speedup of more than two times compared to running on Titan's CPUs alone for that science target.

With his INCITE, CAM-SE and other research work, Norman has become known as a "GPU guy" within the climate and high-performance computing communities: someone skilled at tailoring algorithms to run on a combination of accelerators and CPUs. He doesn't mind the label, but Norman would rather be known for designing and refining scientific computing algorithms to increase efficiency and accuracy.



Contour plot of potential temperature (in degrees Kelvin, with red the warmest and blue the coldest) for a two-dimensional rising thermal in a neutrally stratified atmosphere at high resolution with selective damping to avoid spurious oscillations (leading to the smaller eddies seen in the plot). This test is designed to tell researchers whether their numerical method gives the correct answer before it's integrated into a full climate simulation code.

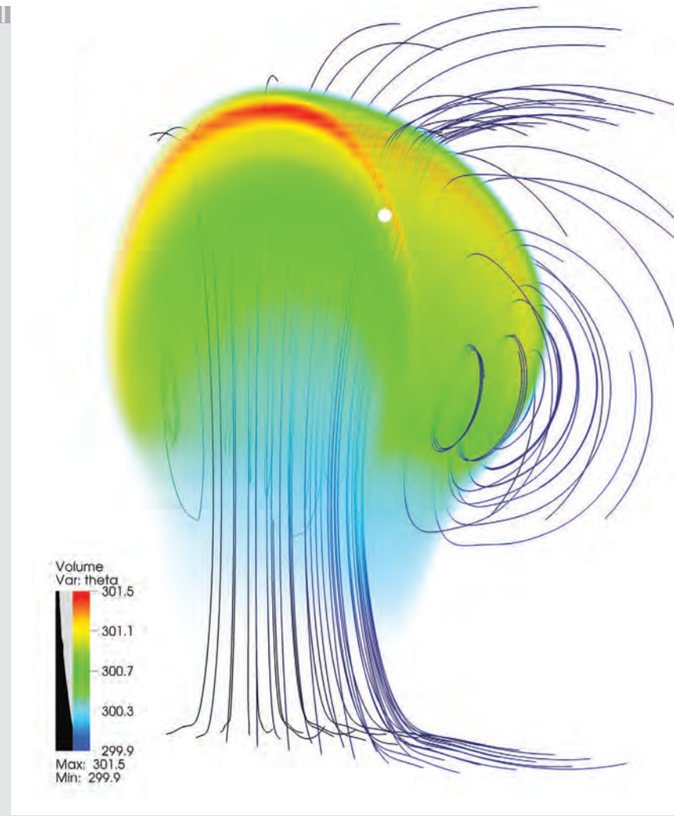
TACKLING A TIME STEP

In one project, Norman addresses a SEM weakness. Compared to other techniques in its class, the method progresses calculations through time in large steps, but the time step gets drastically shorter when calculations are cast in higher-order configurations designed to cut error. "Reducing the time step means it takes longer to get to the final solution, so you want to avoid that."

Norman's modifications to a previously developed technique, however, allow for higher-order calculations without reducing the time step. It's a difficult problem, but "you get a very large time step, very high order, very low communication, pretty much all in one" algorithm. He's demonstrated the method in one-dimensional problems and is working on extending it to two dimensions. That's proven more difficult, he says, but "I've got some tricks up my sleeve."

Norman started as an undergraduate meteorology major at North Carolina State University in his native state and thought he might do television weather forecasting. He soon dropped those plans, however, after discovering he liked math more than meteorology.

When he's not wrestling with algorithms, Norman usually is home with his wife, Shannon, and the latest in a series of foster children they've hosted. While there are challenges in getting children into permanent homes, hopefully with their birth parents, "the reward is just getting to spend life with these great kids," Norman adds.



This test of a climate simulation numerical method shows a volume rendering of potential temperature sliced down the y-axis with streamlines to show wind directions for a three-dimensional rising thermal in a neutrally stratified atmosphere. The colors denote temperature in degrees Kelvin, with red the warmest and blue the coldest. *Images courtesy of Matthew Norman.*

Amoolya Singh
Amyris Inc.

Creating Tiny Factories

IT'S DIFFICULT TO DECIDE what she likes best about her work at Amyris Inc., Amoolya Singh says. There are so many rewarding aspects.

Perhaps it's "the impact and the potential to do something that benefits not only our immediate needs for society, but also might result in a cleaner future" for her twin 5-year-old boys, says Singh, a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient from 2002 to 2006.

Singh heads the Scientific Computing Group at Amyris (pronounced AMerus), based in California's Bay Area. The company engineers microorganisms – mostly yeasts – to ferment sugars for a range of biorenewable products, including drugs, fuels, flavors, fragrances and tire components. Today most such substances are made from petroleum.

"Every kind of plastic and synthetic material that's around you, we may have a hook into making" from renewable feedstocks, Singh says. Amyris believes its products will offer alternatives to many oil-based products within a decade.

PUMPING OUT STRAINS

The scientific challenge also is rewarding, Singh says. The company's automated strain engineering platform pumps out around 30,000 new yeast genotypes per week. Researchers test each strain's fermentation capacity at lab scale, usually in high-throughput plastic plates with 96 300-microliter wells in each. Tests measure the strains' health and viability, what the strains produce, product in proportion to sugar consumed, and undesirable byproducts.

"You can imagine that each strain has multiple measurements taken at multiple points in time, so that's a really massive data set to look through," Singh says. "Using all this information together we can try to predict how a strain would perform at greater and greater volumes."

It's another aspect of her work that Singh prizes. "It's very rare to come across places that have so much data of so many different dimensions and units and to think about how to integrate all that."

Each week, Singh and her team help Amyris biologists decide which of the thousands of new strains should advance to larger-scale fermentation tests. "Running a 200,000-liter fermenter is an expensive proposition," she adds, so getting it right is imperative. Her team uses algorithms that analyze multiple variables simultaneously to infer which properties can best predict how a yeast strain will perform at scale.

"We have databases and algorithms that handle these routinely in almost a touchless fashion," Singh says, but humans also analyze a fraction of the results. "The algorithm has false positives and false negatives, and we can use a hybrid approach with people as well as algorithms" to ensure accuracy. Besides seeking the most promising yeast strains, the researchers also target particular properties, such as yield.

Most of the computations run on the company's in-house Linux machines. The Scientific Computing Group sends more demanding calculations to cloud computing applications. Singh's department divides its time between analysis and devising analytical tools written in the Python, R and F# languages and the SQL database management language.

The most promising yeast strains move on to nine-day fermenter runs at greater capacity. Ultimately the best ones make it to the company's production fermentation facility in Brazil.

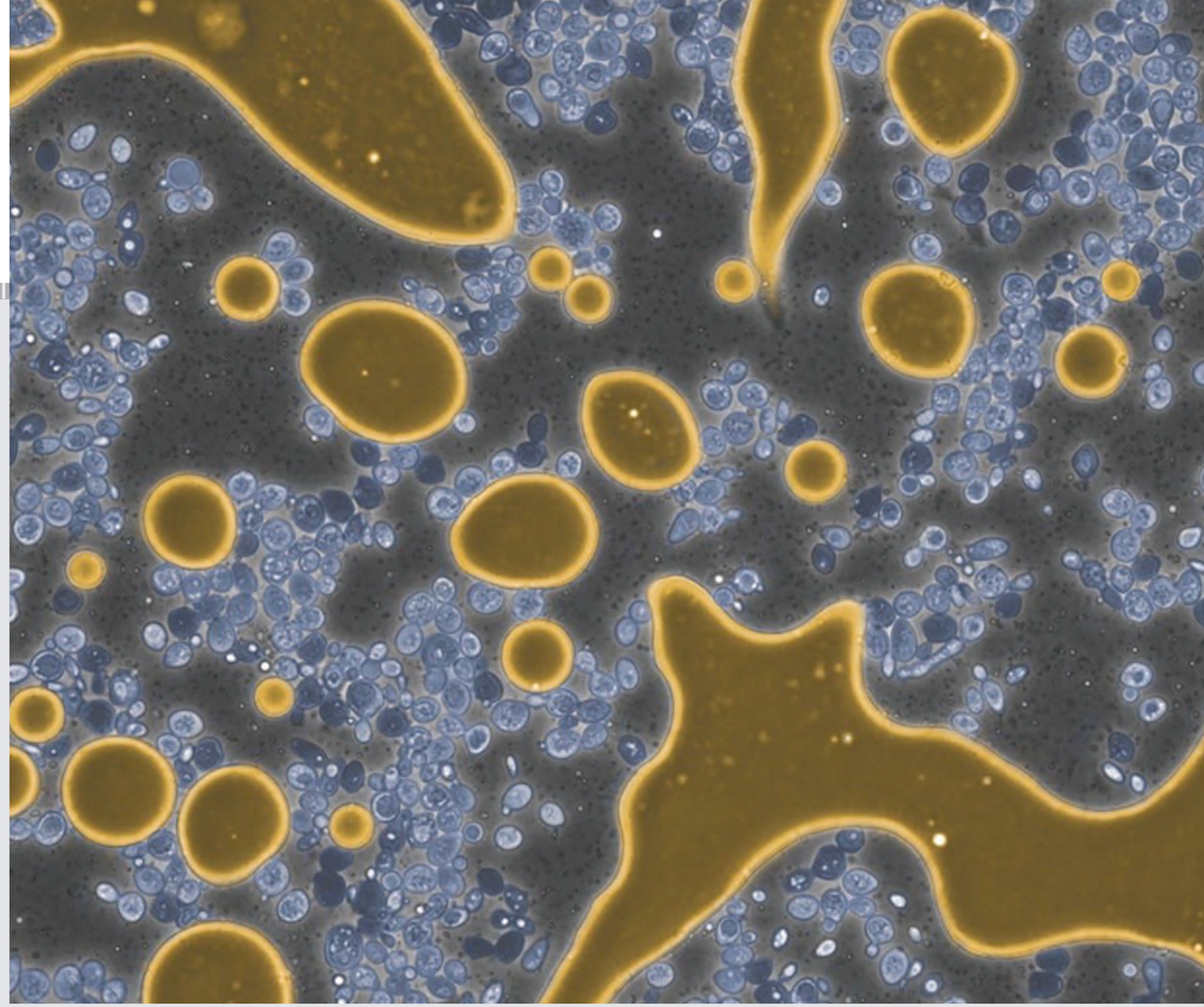
FROM MUSIC TO BIOLOGY

Singh's parents are biology professors in her home country of India, but it wasn't clear she would go into that field. She studied music all her life and pondered it as a profession. She also considered a career in architecture.

In the end, she came to the United States to pursue biology and computer science at Carnegie Mellon University. She later earned a DOE CSGF and graduated with a doctorate in computational biology from the University of California, Berkeley.

Singh credits the fellowship's curriculum requirements with greatly strengthening her training and preparing her for her current duties. She also made many friends with other fellows at the DOE CSGF annual program review, which was "super valuable," she says.

"It was almost a relief to meet other people" who were working at the science-computing interface "and see that we had so much in common."



This microscope image shows Amyris Inc.'s genetically engineered yeast cells producing farnesene, an oily 15-carbon molecule used for making tire additives, lubricants, cosmetics and fuels. The dark brown blobs are farnesene, the bluish granules are yeast and the gray areas are sugar. *Image courtesy of Amyris.*

John Dolbow
Duke University

Extending a Method for Collaboration

WITH HIS BACKGROUND, John Dolbow could define himself as an engineer, a mathematician or a computer scientist.

But the Duke University professor thinks of himself as a computational scientist first, a title that best encapsulates the combination of fields he works in. "On a daily basis, what I am really doing is a mix of engineering, applied math and computer science," says Dolbow, a Department of Energy Computational Science Graduate Fellowship recipient from 1997 to 1999.

Dolbow's unusual appointment at Duke reflects his broad interests. He's in three departments: civil and environmental engineering, mechanical engineering and materials science, and mathematics. That lets Dolbow recruit graduate students from each department for interdisciplinary research.

What connects many of these subjects: the extended Finite Element Method (XFEM), a major computational science advancement Dolbow helped develop as a Northwestern University graduate student. It's become his main tool to investigate phenomena as diverse as fractures, soft-wet materials and the interactions between fluids and structures.

As the name suggests, XFEM is an enhancement of the Finite Elements Method (FEM), a mathematical technique for discretization: the computational process of dividing an object or an area with a mesh of elements so a computer can calculate the physical processes happening in each. When reassembled, the elements portray the entire object or area. It's similar to how thousands of pixels comprise a digital image.

CHANGING GEOMETRY

FEM, Dolbow says, was designed partly "to deal with problems where the geometry was fairly complex," like modeling what happens in engine components. It works best when the geometry doesn't change dramatically. The FEM is powerful, but is limited "when we run into problems where there's an evolving geometry that's central to the problem."

Fractures fall into the problematic category. They have sharp features, they're irregular, and they can break the modeled domain into separate subdomains as time progresses.

In the late 1990s, Dolbow's advisor, Ted Belytschko, and fellow student Tom Black laid the groundwork for what became the XFEM. Dolbow, with postdoctoral researcher Nicolas Moës, worked to make Black's developments simpler for computer scientists to implement.

Finite element users typically shape mesh elements to what they're trying to model. "We came to realize that approach is really very arbitrary — that it wasn't necessary," Dolbow says. He and his colleagues concluded they only needed to ensure the mesh covered the domain under consideration. By adding mathematical functions and modifying the algorithm that integrates the elements, they could model an evolving system, like a widening fracture.

"I think, philosophically, that was a big breakthrough in the way the Finite Element Method was viewed, and it generated a lot of ideas," Dolbow says. The paper that he, Moës and Belytschko published 15 years ago has more than 3,000 citations.

EXTENDING THE EXTENSION

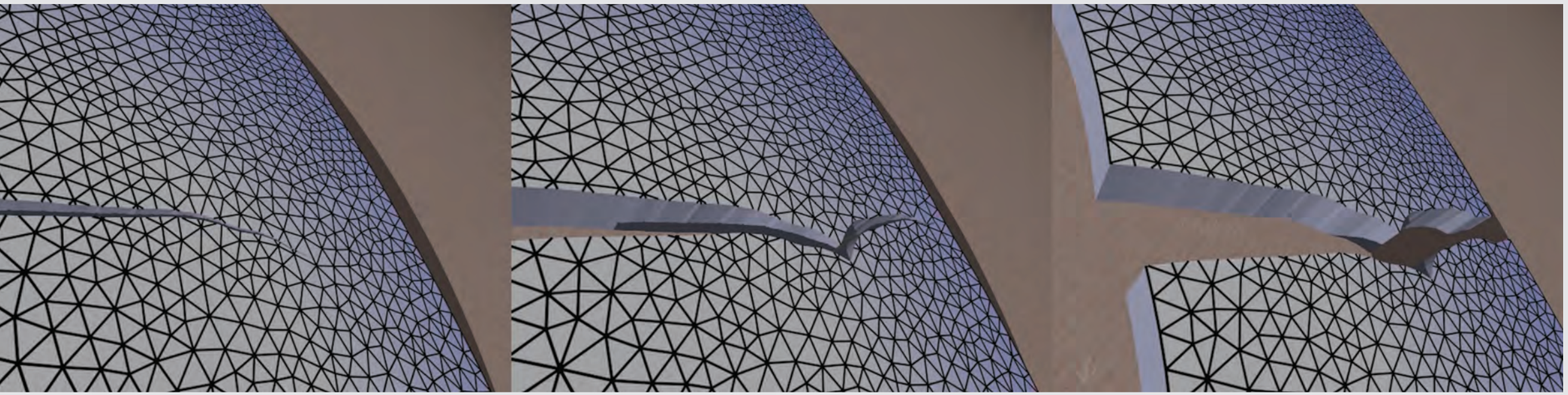
Since then, Dolbow has worked on improving the XFEM and applying it to new problems. He's modeled evolving interfaces, especially boundaries between two material phases, and fluids as they interact with structures.

On a recent sabbatical at Sandia National Laboratories in New Mexico, Dolbow worked with staff members to improve codes simulating large-scale fragmentation. "What I'm interested in are situations in which the loading on the system is very fast," changing it "from a state where things are highly connected to one where things are highly disconnected." It's "a very challenging computational science problem."

Now Dolbow is helping shape the future of computational science in the Department of Energy. He's one of the newest members of the Advanced Scientific Computing Advisory Committee (ASCAC), a group of experts that helps guide the Department of Energy's Advanced Scientific Computing Research (ASCR) program.

The biggest issue confronting the committee and ASCR, Dolbow says, is exascale computing: machines capable of speeds a thousand times faster than today's best. With exascale, the computer architecture that largely sits in the background in developing computational science codes will push to the forefront. Many national laboratories' codes have decades of history, and "one of the challenges is going to be figuring out how best to adapt those to work on exascale platforms."

Dolbow had to call in for his first ASCAC meeting. In fall 2014 he and his family (wife Alice and daughters Zoe, 4, and Maddox, 8) were in Japan to serve the first part of his sabbatical, at the Okinawa Institute of Science and Technology.



Simulation of dynamic crack propagation using the eXtended Finite Element Method (XFEM). *Image courtesy of John Dolbow.*

WINNING CYSE ENTRY

COMMUNICATE YOUR SCIENCE & ENGINEERING CONTEST

ANDREW STERSHIC

BUILDING BATTERIES FROM THE MICROSTRUCTURE UP

RECOGNIZING WRITING SKILL

For 10 years, the DOE CSGF has staged a competition designed to give current and former fellows an opportunity to write about their work with a broader, non-technical audience in mind. The contest encourages communication of the value of computation and computational science and engineering research to society.

In addition to recognition and a cash prize, winners receive the opportunity to work with a professional science writer to critique and copy-edit their entries. This year's winner is Andrew Stershic, a fourth-year fellow in civil engineering and computational mechanics at Duke University.

For more information on the Communicate Your Science & Engineering Contest, visit **www.krellinst.org/csgf/outreach/cyse-contest**.

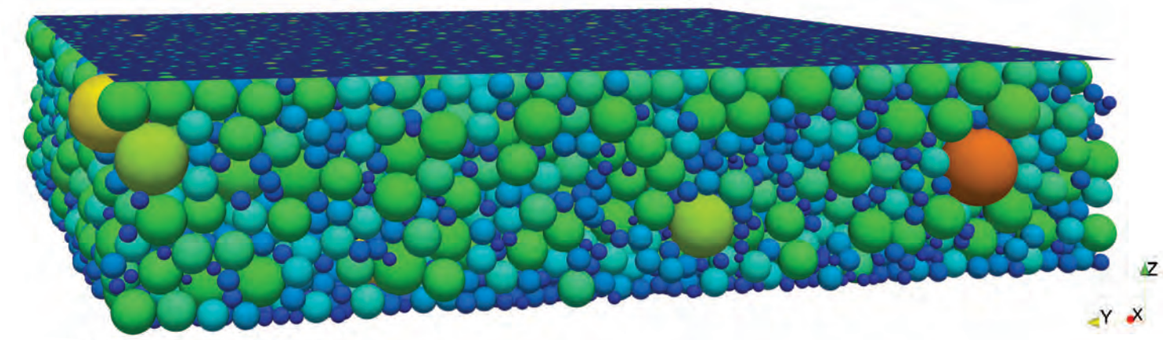
TIRES SQUEAL BEFORE A LOUD crash. Car parts, antifreeze and glittering glass litter the street. An iPad hits a sidewalk. Cracks erupt like a spider web across the device's screen.

We understand pretty well how everyday brittle materials – ones that crack after even tiny deformations – break. But scientists have a hazier picture of another vital fracture phenomenon: how brittle particles in lithium-ion batteries crack. These batteries power our modern world; they are ubiquitous in iPhones and electric cars alike. Their high power and ample charge capacity also make them contenders for large-scale energy storage. For example, Tesla Motors founder Elon Musk unveiled a system in April that can store solar energy in large household batteries to provide power day and night. Electric utilities can use similar devices to make renewable energy a more dependable option for millions of users. The battery market exceeds $100 billion annually, with lithium-ion grabbing an increasing share.

Despite our growing need for them, however, lithium-ion batteries aren't as safe or efficient as they could be. Recall the news stories about Tesla cars erupting into flames after minor collisions? And on a smaller scale, damage during manufacturing robs us of storage performance and prematurely shortens battery life.

What if the same techniques we use to model cracks in glass also could help make lithium-ion batteries safer and more powerful?

The application of a leading fracture model to simulate cracking starting at the corner of a concrete bracket. *Image courtesy of Andrew Stershic.*



A Discrete Element Method simulation of lithium-ion cathode particles as they're pressed during manufacturing. This model captures the motion of every particle but does not describe their cracking or splitting. *Image courtesy of Andrew Stershic, from A.J. Stershic, S. Simunovic, and J. Nanda. "Modeling the Evolution of Lithium-ion Particle Contact Distributions using a Fabric Tensor Approach." Submitted* to Journal of Power Sources.

If we look deep inside them, we can see what's going on. There are two sides, the anode and cathode, represented by minus and plus signs. Each is made of a skeleton of particles, and lithium ions (Li+ for chemistry folks) flow in one direction or the other, depending on whether the battery is charging or discharging. The cathode microstructure is made of millions of spherical particles of a brittle metal oxide containing materials such as lithium, cobalt, nickel and manganese.

The particles must be sandwiched between two metal sheets before the battery can be rolled into the familiar cylindrical shape. They're laid in a wet paste onto the sheet and pressed to the desired thickness.

This is where the problem begins: Because the cathode particles are so brittle, some crack under the pressure. The battery works by exchanging lithium ions between the cathode and anode and sending electrons to the outer plates. When particles crack and split, their interconnectivity weakens. If electrons have a harder time traveling through the cathode skeleton to the outer plate, then the battery doesn't store and supply as much power.

Cracks in the battery particles can get worse as the battery is used. During charging and discharging, the cathode particles correspondingly shrink and grow, causing some small cracks from the initial pressing to enlarge, splitting the particles. This is one reason battery life gets worse with age.

The standard method for computationally modeling battery microstructure geometry portrays each particle individually but at a low accuracy. Because there are millions of them, it's difficult to do more, and so these models imprecisely predict or represent events like particle cracking.

But by using computational failure models that simulate cracks on larger objects – like windowpanes and iPad screens – we can identify and predict loading cases that make lithium-ion battery particles fail. For our study, we have great experimental data of the cathode microstructure at different stages of manufacturing. We're also preparing an experiment to load individual particles and record their failure pressures and crack patterns. Comparing these tests to numerical models helps us fine-tune their input parameters. We can then evaluate how likely specific loads are to crack particles. With this information, we can evaluate alternative materials and manufacturing processes to reduce particle splitting, making batteries more powerful and efficient.

There's a great opportunity to improve lithium-ion batteries by developing and applying numerical models that simulate failure by cracking. This also improves mechanical modeling in a number of fields, enhancing technology development. Creating more powerful batteries will have far-reaching impacts on the consumer electronics and automotive industries of today and will enable development of industries we've never imagined tomorrow.

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.

QUANTUM PRODIGY

MATTHEWS RECOGNIZED FOR LEADERSHIP IN COMPUTATIONAL CHEMISTRY

Devin Matthews of the University of Texas at Austin accepts the Howes award from selection committee chairman David Brown, director of the Computational Research Division at Lawrence Berkeley National Laboratory.

As a high school sophomore, Devin Matthews developed a computer program that attempted to solve the famed Schrödinger equation, which describes an atomic system's quantum mechanical state.

By the time Matthews began at the University of Texas at Austin three years later, he knew more about quantum chemistry than many new graduate students. A chemistry and biochemistry professor, John Stanton, was so impressed he brought Matthews, still just a freshman, into his research group.

Matthews went on to win a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) and to earn a 2014 chemistry Ph.D., with Stanton supervising. His high-precision, high-efficiency algorithms and software are making significant contributions to computational quantum chemistry.

For his technical achievements, leadership and character, a committee of DOE CSGF alumni and friends named Matthews the 2015 Frederick A. Howes Scholar in Computational Science.

Howes, manager of DOE's Applied Mathematical Sciences Program, was an advocate for the fellowship and for computational science. Friends founded the award after he died at age 51 in 1999.

Matthews received his honorarium and award in July at the fellowship's annual program review in Arlington, Virginia.

A COMPUTER SCIENCE INTRO

Matthews now is a postdoctoral researcher in the Science of High-Performance Computing Group and the Institute for Computational Engineering and Sciences at UT-Austin. He says his computer science experience began with his 2011 practicum at Argonne National Laboratory, where he collaborated with Edgar Solomonik, a DOE CSGF recipient now at Switzerland's ETH Zurich. Together, they tackled tensor contraction, a common operation found in quantum chemistry calculations, especially methods known as coupled cluster. Tensors organize data with multiple dimensions. For example, a matrix is a two-dimensional tensor.

Quantum chemistry is key to understanding the details of atomic and molecular interactions. Coupled cluster methods describe these complex many-body problems, in which particles – electrons, in this case – influence each other. The methods yield an approximate solution to the Schrödinger equation.

At its highest level, Matthews says, computational chemistry captures the details of atomic and molecular interactions, including electron arrangements, as accurately as experiments. But "those are heavyweight calculations. In the future the idea is to exceed the accuracy of the experiments or to do calculations where we simply can't do an experiment yet – to be really predictive."

Matthews and Solomonik, with Argonne intern Martin Schatz, devised the Cyclops Tensor Framework (CTF), a method that exploits symmetries in tensor data to perform contractions more quickly and efficiently than other approaches.

Cyclops plays a role in one of Matthews' latest projects: Aquarius, a framework for quantum chemistry tensor computation. The idea is that "if you have very efficient tensor contraction, you can make everything efficient across the board by simply plugging" in that method, Matthews says.

In most cases, quantum chemistry programs include code for all operations, including tensor contraction. Aquarius users, however, can plug in a tensor contraction method they believe is best or more useful for a specific application. Aquarius uses CTF, Matthews says, but he's working to support other techniques.

INTERCHANGEABLE EMPHASIS

Researchers are using Aquarius, but Matthews also wants them to embrace its approach. "If people adopted the philosophy I've put into it and make software work together and be interchangeable, that would be a really positive impact" on computational science.

In its citation, the Howes selection committee wrote that Matthews' leadership on Aquarius "speaks highly to his willingness to challenge the bounds of state-of-the-art in computation, to take responsibility, and to follow through with dedication and drive."

Matthews also has distinguished himself as a mentor and leader, the committee noted, by initiating projects and supervising and assisting fellow graduate students and colleagues. "Devin's demonstrated excellence in research and leadership in the computational quantum chemistry community exemplifies the qualities that Fred Howes encouraged in all young scientists," the citation says.

Matthews' accomplishments have opened numerous career opportunities. He finds academia the most attractive but would consider an industrial post. A desire to be near family in the Austin area also will influence his choices.

Regardless, Matthews says he'll continue supporting the DOE CSGF. His advice to new recipients: Maximize the program's features. "It's not just paying a stipend and paying your tuition. It's giving you opportunities to make connections and do new things and learn to work with people from other fields."

ABOUT FRED HOWES

In the 14 years since it was first conferred, the Frederick A. Howes Scholar in Computational Science award has become emblematic of research excellence and outstanding leadership. It's a fitting tribute to Howes, who was known for his scholarship, intelligence and humor.

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

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

PAST HOWES SCHOLARS

2014	Hayes Stripling IV
2013	Ashlee Ford Versypt
2012	Carolyn Phillips and Matthew Reuter
2011	Alejandro Rodriguez
2010	Julianne Chung
2009	David Potere
2008	Mala Radhakrishnan
2007	Jaydeep Bardhan and Kristen Grauman
2006	Kevin Chu and Matthew Wolinsky
2005	Ryan Elliott and Judith Hill
2004	Collin Wick
2003	Oliver Fringer and Jon Wilkening
2001	Jeffrey Hittinger and Mayya Tokman

FELLOWS: MAJOR DISCIPLINES

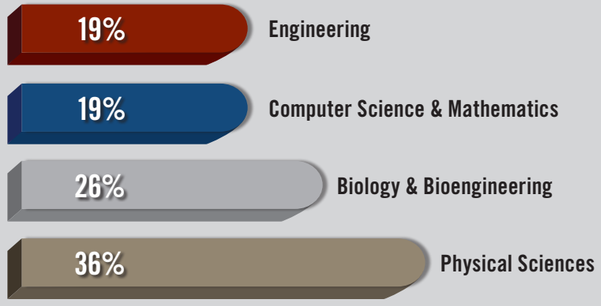
Students who enter the Department of Energy Computational Science Graduate Fellowship must combine courses in applied mathematics and computer science with courses in specific application disciplines, preparing them to apply high-performance computing in a range of fields. The accompanying graphic groups fellows into four broad areas, but they study a diversity of specific subjects.

Graduates go on to take leadership positions in industry, academia and government laboratories, helping the United States address vitally important problems.

The DOE CSGF is supported by the DOE Office of Advanced Scientific Computing Research (ASCR) within the Office of Science and the Advanced Simulation and Computing (ASC) program within the National Nuclear Security Administration.

For complete lists of fellows and alumni (by last name, Ph.D. institution, fellowship start year, practicum location, current location and area of study), go to **www.krellinst.org/csgf.**

DOE CSGF FELLOWS: DISTRIBUTION BY DISCIPLINE*



*For 2014-15 Academic Year

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Not pictured: Will Fletcher, Ryan McKinnon, Thomas Thompson and Alexander Williams.

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