DEIXIS (ΔΕΙΞΙΣ) transliterated from classical Greek into the Roman alphabet, (pronounced daíxis) 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. DEIXIS illustrates work done at eight multi-program DOE laboratories and 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.
FOR OVER 10 YEARS, the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) program has been providing support to the nation’s best new scientists. The DOE CSGF program’s innovative requirement of cross-disciplinary study in science, engineering, applied mathematics, and computer science sets it apart from any other fellowship program in the country.

University of Washington | Lawrence Berkeley National Laboratory | Story
by Jacob Berkowitz

Mary Ann Leung told her house, quit her successful 16-year-long career as a trainer and instructional designer in the computer industry, and, at age 38, returned to college to become a physician. Or so she thought. On her way to the medical sciences she discovered a long unrealized passion for math and the computational sciences. Now a Department of Energy Computational Science Graduate Fellow (DOE CSGF), she is using high-performance computing to understand the role of quantum mechanics in applications ranging from nanoscale engineering to the emerging field of quantum computing.

In 1997, Mary Ann Leung found her groove during a National Science Foundation-sponsored undergraduate-summer stint in the lab of Dr. William (Bill) Reinhardt, a University of Washington professor of chemistry and adjunct professor of physics.

“I fell in love with the work I did,” says Leung, now a third-year doctoral student in Dr. Reinhardt’s lab at the University of Washington. Her job that first summer was to develop a computer program to visualize the time propagation of solitons in the Bose-Einstein Condensate (BEC). While planning a slide presentation of her work, she came across an image of a BEC generated by one of Dr. Reinhardt’s computer programs. It was a moment of scientific and personal epiphany.

“The image had a strong likeness to a piece of artwork that I’d created 20 years earlier. I decided at that point that I’d been visualizing math much earlier in life, but I just hadn’t realized it. So, seeing this image made me feel like I’d found my calling,” recalls Leung.

Ironically, she returned to school several years earlier she would never have seen her calling. In 1993, Albert Einstein and Satyendra Nath Bose hypothesized that noninteracting atoms chilled to supercold temperatures (about 190 nanoKelvin) would condense into a new form of gaseous matter, the BEC. What’s remarkable about the BEC, they explained, is that in this supercold state the atoms would all go into the same quantum state: They would behave as a single super atom, a macroscopic quantum object large enough to be visible to the naked eye.

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However, it wasn’t until 1995 that three independent research teams were succeeded in creating the first BEC by supercooling rubidium-87, lithium-7, and sodium atoms. This breakthrough has set off a global wave of experimental work with BECs.

“They’re a wonderful place for people to explore the fundamentals of quantum mechanics because you can see the quantum effects,” says Leung, noting that BEC research has applications to fields ranging from superconductivity to nonlinear optics.

In the process of her doctoral work, initially focused on developing parallelized codes to understand and visualize the dynamics of solitons and vortices in BEC, Leung found her own kind of quantum coherence—a fellowship program that was just right for her.

“When I found the DOE CSGF, I thought: This is perfect for me. I love all of these things,” recalls Leung. The Fellowship requires participants to take science, applied math, and computer science courses, and Leung was particularly inspired by an algorithms course.
For over 10 years, the DOE CSGF program has encouraged the training of computational scientists by providing financial support to some of the most talented graduate students in the nation. Phase II for the fellowship appeared in the National Science Foundation's Division of Mathematical Sciences publication Mathematics and Science.

Leung and Canning's simulations have already provided a more detailed physical understanding of the nickel-copper quantum well state experimental results, as well as confirming some of the theoretical models used by Dr. Qiu's group.

Leung says that it was great to work closely with Dr. Canning and his post-doctoral student in a "collaborative environment that was really about pursuing interesting science." The experience provided Leung with a clearer sense of her potential.

"One of the important lessons that I learned from that experience was that you can apply yourself to a new field and within a relatively short amount of time, you can learn quite a lot and make progress," she says.

It is a lesson she has taken back to her doctoral research at the University of Washington. Along with her supervisor Dr. Reinhardt, Leung is exploring the potential of the BEC and high performance computing for the study of quantum computing.

Amidst the enormous international scientific buzz about quantum computing, Dr. Reinhardt is cautiously optimistic that BEC research offers a unique approach.

"Because BECs are big and you can control them with lasers, we're trying to figure out if we can use these very special macroscopic properties to make extra-stable pieces of quantum computers," he says, noting that as a large quantum object the BEC might be less prone to the quantum decoherence that disturbs single atom quantum computing systems.

At the same time as she is working towards numerically modeling a quantum computer, Leung is also helping others push scientific boundaries. She volunteers with organizations dedicated to encouraging girls to study science and engineering.

"In high school, I realize that I was always really good in math when I was a kid," says Leung. "But I never really received any encouragement to do anything with math. Quite the contrary, I was discouraged: 'That's not a girl thing to do.' Since I got such a late start in science, I really want to encourage young girls and women to go into science; it's a fascinating field."

For more information on the DOE CSGF, prospective students are encouraged to visit the website at http://csf.lbl.gov/.
A lot of graduate students tend to fall into this dynamic where they’re looking just at their one research problem and lose perspective on what’s happening in the whole field that they’re working in. There’s a larger world out there than the one little problem that you’re trying to answer.

Challenge of Simplification

AHMED ISMAIL
Massachusetts Institute of Technology
Oak Ridge National Laboratory
Story by Jacob Berkowitz

Simplify. It’s a way of being for some people. To rid themselves of clutter, they remove all that’s non-essential so as to be left with the key elements of life. For Ahmed Ismail it’s the key to his research.

This computational minimalist spends his days trying to remove everything that’s numerically extraneous, honing codes and algorithms until he’s left with a gleaming gem of Truth.

The challenge is how to get to this place of computational enlightenment. While the goal is to simplify, the route there involves numerous complex steps. For Ismail, his journey to greater place of computational enlightenment.

“Polymers are perhaps the largest and fastest growing area of materials for engineering applications,” says Dr. Gregory Budilige, Director of MITE’s Program in Polymer Science and Technology, and one of Ismail’s co-advisors. “The development of advanced, atomically detailed modeling methods is crucial to determining the molecule-sized origin of a wide spectrum of polymer properties.”

Ismail’s doctoral research has focused on the use of position-based coarse-graining to simplify a range of chemical problems. Beginning with the simulation of living models, lattices of magnets, 250,000 atoms, you’ll never finish your simulation. However, for most of the properties that you want, you don’t need to worry about the position of every single atom and electron. You just need to know the basic average properties of the system.

To accelerate the calculation of these average properties, Ismail uses a multiresolution technique called the wavelet transform. This mathematical tool acts as a filter through which data can be recursively processed until it meets thousands of variables into a single average value.

Winning. This process of simplification can follow Ismail’s doctoral work on coarse-graining time-based or position-based. While both methods are designed to reduce the number of variables or degrees of freedom in a simulation, in practice they are significantly different.

Ismail’s doctoral research has focused on the use of position-based coarse-graining to simplify a range of chemical problems. His basis is a multiresolution technique called the wavelet transform. To accelerate the calculation of these average properties, Ismail uses a multiresolution technique called the wavelet transform. This mathematical tool acts as a filter through which data can be recursively processed until it meets thousands of variables into a single average value.

From my point of view it was a significant differentiator in this field, recalls Ismail. “If you’re in industry and you’re looking at my tiny niche problem, you will very quickly give you an order-of-magnitude estimate for where this behavior is going to occur,” says Ismail.

However, his contented path to simplification took an abrupt turn last year when he received a call from Dr. William Shelton, a Senior Research Staff Member in the Computational Materials Science Group at ORNL, inviting Ismail to do his post-doctoral work in Oak Ridge, Tennessee.

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Dr. Shelton’s project (prompted by Dr. Shelton’s work in Polymer Science and Technology) was one of a dozen people in his group who were looking at new and efficient approaches to polymer models. As I'm going to experience, says Ismail. “There is a lot out there on how to do coarse-graining, but right now a lot of it is on an academic level. People pick a particular model because it works, but we need to develop strong first principles approaches and a systematic method for choosing how to simplify them.”

Program

Since its inception, the DOE CSGF program has supported 244 students in over 50 universities all over the U.S. Currently it supports nearly 75 students in 21 states: Arizona, California, Georgia, Illinois, Indiana, Iowa, Massachusetts, Michigan, Minnesota, New Jersey, New Mexico, New York, North Carolina, Oregon, Pennsylvania, Tennessee, Texas, Utah, Virginia, Washington, and Wisconsin.

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Thinking Small to Predict Large-Scale Turbulence

RANDALL MCDERMOTT

University of Utah - Sandia National Laboratories - California | Story by Lori Valigra

Are the interpolated experimental data. The lines connected by dots are results of the large eddy ODT and data to the left is from LES. The dotted line furthest left represents the wavenumber of the Navier-Stokes equations of the combined LES and Comte-Bellot and Corrsin isotropic turbulence which the LES and ODT are joined. In other words, the largest allowed eddy in the ODT model.

The stimulus behind his move for a DOE CSFG fellowship was a desire to apply his background in practical, applied engineering to theoretical problems. “That led me back to school,” said McDermott. “I realized while working at Zink that I needed a bigger tool box to tackle the types of problems encountered in combustion applications.” For McDermott, the practicum took five months, and led him down a path that he and his advisors at Utah and Sandia changed his research focus for the better.

Combustion is really fun. In one way or another it touches on every aspect of chemical engineering.” His advisor at the University of Utah, Philip Smith, encouraged him to take the DOE CSFG fellowship. Prof. Smith was on a roll; McDermott is the second of his graduate students to be honored with the prestigious fellowship. Diem-Phuong Nguyen, highlighted in Diex last year, graduated from the program in 2005. Her fond experiences likewise motivated McDermott to pursue the DOE fellowship.

When it came time to choose a practicum site, Randy chose Sandia National Laboratories in California. “Choosing the practicum location was not easy at all. I had boiled it down to the Bar area. In the end, our group at Utah has close ties with Sandia. But, I really don’t think I could have made a bad choice.” For McDermott, the practicum took five months, and led him down a path that he and his advisors at Utah and Sandia changed his research focus for the better.

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DOE CSFG HIGHLIGHTS

- Payment of tuition and required fees
- Yearly stipend of $20,000
- A $1,000 allowance for related expenses
- Matching funds of up to $2,500 for a computer workstation
- Opportunity to complete a practicum working with scientists and researchers at a DOE Laboratory
- Yearly fellowship conference with opportunities to meet other fellows and industry and government professionals
- Renewable up to four years

For more information: www.braud.in.gov/CSFG

HIGHLIGHTS
He has chosen the most ambitious goal possible. He’s both-minded and flexible, and is always pushing beyond what’s known.”

Kerstein said McDermott is very well versed in the field of science like simulation, which is very different from traditional science in that it uses an inductive approach, as opposed to a deductive approach, to explain experiments. “We are trying to find a set of equations for turbulence that will work in different applications,” Kerstein said. “Randy has had a very valuable learning experience. He’s built a new model from the ground up.”

McDermott’s relentless efforts in the lab have impressed both of his advisors. “Randy is very focused on what he wants out of his research and what he will get out of an educational experience. He very much wants to know how theoretical science can be applied to real life,” said Smith.

“Randy has special qualities. He takes weaknesses of the problem,” said Alan Kerstein, McDermott’s practicum advisor at Sandia. “He’s not looking to narrow the focus to the smallest specialty as students often do to define a problem they can cope with. He is thinking broadly.

Simulating the Heart

BOYCE GRAFTH
New York University - Lawrence Livermore National Laboratory - Story by Lori Valgus

When New York University mathematics student Boyce Griffith embarked on a cross-country car trip to California’s Lawrence Livermore National Laboratory (LLNL) last year, he had only a hint of the ambitious research projects that ultimately would take place during his DOE CGSF fellowship pursuit.

Now preparing for his second practicum at LLNL, Griffith plans to build on his earlier work of developing software for large, parallel computers that aim to simulate the heart and solid structures interact within large physiological systems, and get it to work on a three-dimensional model of the heart. The result might be a better understanding of heart problems, such as arrhythmias and sudden cardiac death, which cause about 500,000 deaths yearly in the United States alone.

Heart disease remains one of the leading causes of death in developed nations, and it can only be treated after an event occurs. “We need to obtain experimental measurements much beyond the surface of an intact heart,” Griffith said. “The results we obtain from numerical simulations of turbulence will work in different applications.”

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McDermott’s relentless efforts in the lab have impressed both of his advisors. “Randy is very focused on what he wants out of his research and what he will get out of an educational experience. He very much wants to know how theoretical science can be applied to real life,” said Smith. As a problem arises, the students will be required to define the scope of the problem, with some additional electrical modeling, during his second practicum.
Unfolding Proteins

PROTEIN FOLDING

Understanding how a string of amino acids, each with its own unique chemical and physical properties, folds up to form a fully functional protein has presented a formidable challenge for decades.

In fact, just as a whole branch of mathematics is devoted to the study of origami forms, the challenge of protein folding has engendered an impressive array of mathematical models designed to predict protein folding behaviors. And with the avalanche of DNA and protein sequence information being generated by genomics and its counterpart, proteomics, the rush is on to convert that data into information about fully functional folded proteins.

Solving protein structure requires a combination of knowledge from physics, biology, chemistry, and perhaps the most limiting factor: massive computational firepower.

“High performance computing has transformed our ability to take on the challenge of global energy minimization,” says Teresa Head-Gordon, assistant professor of Bioengineering at the University of California at Berkeley.

“Back in a 1972 Nobel Prize-winning theory developed in the late 1960s by Chris Anfinsen of the National Institutes of Health, which stated that the three-dimensional structure of a protein is the one in which the free energy is at its lowest. The free energy takes into account the watery environment of the protein and all the various atomic interactions of the amino acids. Since these initial experimental insights, scientists have discovered that proteins fold into three-dimensional shapes that include a limited number of preferred configurations that define their secondary structure. These shapes include alpha helices, beta pleated sheets and various types of coiled loops. The final folded protein may bring amino acids that are far apart from each other in the starting amino acid chain close together, just as, in the creation of an origami swan, opposite corners may end up folded together.

Tackling the limitations of movement imposed by the protein’s chemical components still creates a mathematical origami that can tax the capacity of even the powerful parallel computers available at LBNL.

“High performance computing has transformed our ability to take on the challenge of global energy minimization,” says Head-Gordon. “We had to start with an initial structure in order to search the possible conformational states,” Head-Gordon says. “We have to have secondary structure already formed to do global optimization. We were using local optimization with some constraints to form that secondary structure. It took hours or days of computational time to get those structures formed.”

“Then Crivelli brought in a mathematical representation of origami, a mathematical representation of origami that allows a user to experiment with various protein conformations before settling on a ‘best guess,’ which can then be subjected to rigorous global optimization algorithms. Just as in the cell, amino acids are added to the structure one at a time. As the protein grows, the program searches through a database of known protein structures, manipulating long strings of amino acids without ‘breaking’ them.”

Crippelli’s idea was to be able to manipulate long strings of amino acids without “breaking” them.

To solve the problem, Crippelli sought a way to cut the time needed to reach a reasonable secondary structure, one that incorporated all the likely alpha helical regions and beta sheets, to an hour or two. Rather than using time-consuming local optimization methods, she sought to create a tool that would allow a user to experiment among various potential conformations while simultaneously monitoring the energy profile of the protein.

They took advantage of a technique called “inverse kinematics,” which calculates the movements of several articulated joints at once to reach a desired point in space. The method is used in both computer gaming and robotics to make a character’s movements on screens as natural as possible. For example, it allows a virtual swan to bend its neck in a realistic way.

“In robotics,” Crivelli explains, “when you move an arm, all the joints move. Our problem was similar except we wanted 80 or 90 joints.”

The result is called “ProteinShop,” an interactive computer visualization tool that allows a user to experiment with various protein conformations before settling on a “best guess,” which can then be subjected to rigorous global minimization algorithms. Just as in the cell, amino acids are added to the structure one at a time. As the protein grows, the program searches through a database of known protein structures.
Silvia Crivelli has spent over ten years developing software in high performance computing. She currently works as a Staff Scientist in the Computational Research Division at LBNL, and as a Visiting Associate Research Engineer at the California Institute for Quantitative Biomedical Research at the University of California at Berkeley. She received her BS in mathematics from the Universidad Nacional del Litoral, Argentina, and both her MS and PhD in computer science from the University of Colorado at Boulder.

Further Reading:
S. Crivelli, D. Kropey, N. Mao, and W. Bethel (2003). ProteinShop: A Tool for Interactive S. Crivelli and colleagues are busy designing ProteinShop to allow researchers to adapt it to their various needs.

“If we had a basic understanding of the functional properties we want,” says Head-Gordon. “Predicting beta sheets is more complicated than alpha helices. In CASP5 we will not only compete against the whole spectrum of proteins, including those with high beta content and very difficult topologies. We learned that our infrastructure is solid.”

In particular, colleagues and competitors alike were uniformly enthusiastic about the potential of ProteinShop to become a universal tool that can be applied to many different protein folding methodologies.

to account the forces on each atom and calculates each atom’s position as forces are applied over time. In addition, the team uses a global optimization approach called stochastic perturbation that draws on secondary structure patterns to provide guidelines and hints for the optimization method. The process is repeated many thousands of times until a calculation settles on the most stable configuration.

Complicating the analysis is the difficulty of calculating the energy of a protein chain in the watery environment of a living cell. Head-Gordon’s latest algorithm, which models proteins in water, takes into account the natural tendency of fatty (hydrophobic) amino acids to cluster together, just as oil droplets converge in a pot of water.

The team’s approach was put to the test when they participated in a biennial competition that pits various modeling strategies against one another in a head-to-head competition to predict structures of proteins whose three-dimensional shape is unknown. Teams competing in the Critical Assessment of Techniques for Protein Structure Prediction, or CASP, are given only the amino acid sequence and a deadline for producing a predicted protein structure.

Simultaneously, structural biologists are busy designing protein structures experimentally using X-ray crystallography and other techniques that form a picture of the protein’s actual shape. When the competition is over, the structures are revealed and competitors are rated on how well their predictions conform to the actual protein structure.

“It’s like drinking from a fire hose,” says Head-Gordon. “The deadlines just keep coming and the deadlines are a matter of a few weeks. It really taxes your resources.”

In the most recent competition, CASP5, held in the spring and summer of 2002, the LBNL team, which also includes Bobby Schnabel, Richard Byrd, and Betty Eskow from the University of Colorado, tackled 20 proteins for which no tertiary structure information was available. These proteins, called “new folds,” are the most difficult to solve.

When the initial results were revealed in a December 2002 meeting held at Alamosa, Colorado, Head-Gordon’s team had placed between 13 and 15 out of nearly 200 participants.

“I was very proud of our effort,” says Head-Gordon. “Predicting beta sheets is more complicated than alpha helices. In CASP we will not only compete against the whole spectrum of proteins, including those with high beta content and very difficult topologies. We learned that our infrastructure is solid.”

In particular, colleagues and competitors alike were uniformly enthusiastic about the potential of ProteinShop to become a universal tool that can be applied to many different protein folding methodologies.

would give us the ability to create new materials that are inspired by nature but that nature never thought to make . . . or we could design new materials with the structural and functional properties we want.
QUESTION: What do an aircraft carrier, a submarine, a nuclear weapon, and a miniscule gear (many of which could fit on the head of a pin) have in common?

ANSWER: Salinas's considerable capability allows it to be used to model numerous "what if" scenarios without having to conduct actual nuclear tests.
GARTH REESE

Earth Reese received his BS in physics from Brigham Young University in 1981 and his PhD in physics from Arizona State University immediately following graduation. He began work at Motorola in Scottsdale, AZ, where he designed and analyzed surface acoustic wave filters and resonators. In 1988 he began working at Sandia National Laboratories, doing device development and modeling of piezoelectric components. Since 1991, he has worked in the structural dynamics, analysis, system identification and health monitoring area. He has expertise in development of structural system identification software for reconstitution of finite element structural dynamic models with test results. He is a principal author of Sandia’s Virtual Environment for Optimal Test.

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Mauri K. Eklund

Mauri K. Eklund received his BS, MS, and PhD in aeronautical engineering from Virginia Tech. Immediately after receiving his PhD, Mauri started work in the Structural Dynamics group at Sandia. He has been part of the Salinas team for six years.

Contact: Earth Reese
garthreese@sandia.gov

PRACTICUM COORDINATORS

Albuquerque - Marcus Martin mmarin@sandia.gov

Livermore - Paul Nielsen paulniel@sandia.gov

anti-ballistic missile as it hurls toward its target, or the consequences of a fracture or break in multiple nuclear weapons are launched and one is detonated near another.

"Simulation gives a fair better understanding of what’s happening in these situations and the data is far more complete than could be derived from real tests," says principal investigator Reese. This data can include information not only about whether a weapon will fail or not, but even more specifically about which parts are susceptible to failure. To do this, Salinas shows how the combined wave generated by a strike on a weapon would be propagated from the weapon and to the various inner components. In fact, the program gets so specific, “I can see what particular delamination is going to break,” notes Reese. “The intent is to learn how to design the structure so it will stand up to a certain level of attack.”

Sea and Battle worthy

Similarly, the goal of the aircraft carrier analyses is to aid designers in creating the most seaworthy and battle worthy ship possible while it is still on the drawing boards. Thus can eliminate a lot of trouble and expense, such as that which was incurred when an early carrier was found to ride too high in the water, which was caused by the weight of the ship’s gear, including the large horizontal plates that huge horizontal plates that..." says principal investigator Garth Reese. Hence, “understanding the structure so it will stand up to a certain level of attack.”

Salt of the Earth

Following a tradition among Sandia computer scientists, the Salinas code was named after a local pueblo. The nameake for this program is a pueblo on the east side of New Mexico’s Sandia Mountains. Salinas is also the Spanish word for salt, and, says Reese, “While structural dynamics is not as flashy as in analyzing parts falling off a structure, or studying a large reef, it is crucial for the success of any structure. It is the bread and butter, or the salt. It is the kind of downhill work that things you have to have to get the analysis done for any system.”

Studying the effects of air blasts is part of the recent expansion of Salinas to include the analyses of fluid action, in addition to the structural interactions it was originally designed to study.

In the case of the MEMS gears, the fluid in question is air, which can have a deleterious effect on the gears if they strike 50,000 cycles per second. “A MEMS gear can be designed to run for a long time but may not, because air can erode the energy out of the structure,” explains Reese. Hence, the goal is to understand the interaction between the air and the structure and how the structure behaves as water. Knowing how the structure responds, and how the ping reflects back out, are key to being able to design stealthy substructure.

Fluid structure interaction analysis is also important to the full-scale design of very small parts like the microelectromechanical (MEMS) gears, which may someday find their way into nuclear weapons. These gears can be built into integrated circuit chips, enabling them to operate in concert with microelectronics systems.

And what the salt does is make Salinas scalable. “This means that if you take a model with one million different pieces in it and run it on 500 processors, and then take that model that is twice as large and run it on 1,000 processors, we get the solution just as quickly in either case,” says Reese.

On the surface it seems obvious that if a problem is made 50% more complex, and 50% more processors are used to solve it, then the time required to achieve the solution to both problems will be the same. But when it comes to scalability of computational equations on parallel computers, each running logic does not apply. In fact the reverse can be true — more processors can slow down the speed of calculation. This is so for two reasons. One is that the more processors you put in one another, or spending too much time in communication.

And therein lies the beauty of the linear solver — the result of a collaborative effort between Sandia and the University of California, Berkeley, which restores logic to the world of computing by breaking scalability. And it is that scalability that allows Salinas to run equations on thousands of processors simultaneously, which allows quickly and accurately analyze aircraft carriers, submarine gears, and anything in between.

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Futuristic Fusion

By Peter Gwynne

Scientists have tried for half a century to tame the type of energy that makes the Sun shine. The process, called nuclear fusion, occurs when two atomic nuclei overcome the usual force of repulsion and slam together in a collision that creates a single, heavier nucleus and an excess of energy. The most common form of fusion involves isotopic forms of hydrogen, the simplest and lightest element in existence. When nuclei of the hydrogen isotopes deuterium and tritium collide, the impact creates a nucleus of helium, the next simplest element, and produces enough energy, in the case of the Sun, the force of gravity holds together the Sun and its great radii, to support life on Earth.

On Earth itself, that same process produces enough energy, in the case of the Sun, the force of gravity holds together the Sun and its great radii, to support life on Earth.

The fusion power that makes the Sun shine relies on more than experimental devices. A group at the Oak Ridge National Laboratory is using computer simulations to design a futuristic fusion reactor.

In strictly layman’s terms, computer simulation helps to compensate for a fundamental difficulty of research on plasmas: containing the material. No solid can hold them, because plasmas exist at temperatures far above the melting points of all known materials. That leaves magnetism as the only practical means of keeping plasmas in place. Creating the necessary magnetic fields is both complicated and expensive, however. Thus, the more research scientists can do with computers, the faster their projects will advance.

Batchelor’s group has three main objectives. “First,” he says, “we want to understand the physics of plasma. Second, we are developing computational tools to ask questions, find the solutions and what they mean. Experiments give you a lot of data but don’t tell you what the data mean; we use our computer codes to find the solutions and what they mean.”

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In strictly layman’s terms, computer simulation helps to compensate for a fundamental difficulty of research on plasmas: containing the material.
Don Batchelor's arrival at the Oak Ridge National Laboratory 25 years ago to work on plasmas represented a return to his geographic and scientific roots. He was born at Oak Ridge during the Manhattan project, and the electric fields he created in his mathematics from MIT, he returned to the world of fusion, taking a PhD in plasma physics from the University of Maryland in 1978. At that point, he recalled, “I had a very large, very active theory group at ORNL doing very interesting things, including an absurd experiment called the ELMO tumour, a device driven by plasma waves. So I came to Oak Ridge with the idea here was studying plasmas which was more qualitatively, I got into that work. I’ve been here over thirty.”

Tough Challenges
Understanding the basic physics of plasmas presents a series of tough challenges. “Here at ORNL, we have two teams studying waves and heating in plasmas; the work is very complicated geometrically so that there’s very little you can do with pencil and paper,” says Batchelor. “The most complex research involves understanding how turbulence within a plasma causes the system to lose energy, and hence perform less efficiently than it should.”

“Understanding turbulence is a very difficult nonlinear problem. It’s difficult to work out even for normal liquids, as the pressure goes up, the stability of a fluid can be much smaller but can still have good confinement and stability,” he says. “It has the unusual property that, as the pressure goes up, the stability and the ability to hold the particles gets better.”

To indicate the size of a stellarator, physicists use a criterion called the aspect ratio. “That is the ratio between the largest to the smaller in the magnetically shaped plasma. The best example of a traditional stellarator, a machine called the W7X, now being built in Germany, has an aspect ratio of 11. ‘Ours has an aspect ratio of 3,’ says Batchelor. ‘We’re looking at a tricycle rather than a bicycle tire.’”

The group’s scientists used their theoretical understanding and experience of the technology to come up with a geometry that’s feasible to build.

Finding Funding
As they continue to refine their simulations, the ORNL team has also involved itself in politics and economics. “We’re trying to get funding to build our stellarator,” Batchelor says. For that effort, outside help is available. The team is designing two stellarators — one for the Princeton Plasma Physics Laboratory and the other for ORNL.

To run the software, ORNL’s Center for Computational Science offers four massively parallel computers that can work on several different calculations simultaneously. Batchelor’s team can also call on external computing power. “Our access to big computing here in the Department of Energy has been essential,” he says. “But it doesn’t matter where the computers are: All our studies have made a lot of use of external computing power at ORNL.”

We also use the increasingly powerful computing resources in our department. We have a new Gray vector processor, and are expecting more within the next year. Batchelor wouldn’t object to extra hardware. Asked how much computing power his group needs to carry out its research, he responds: “How much have you got?”

Stellarators created to date have suffered one significant drawback; they have had to be huge in size to be able to hold in the energy and particles that make up plasma. The team also collaborates with the University of Montona and with stellarator teams in Germany and Japan. And the fusion program as a whole involves several other groups at ORNL, including physics, fusion materials, and engineering.

The path to commercial fusion
In the 1970s, physicists working on fusion anticipated that, with an appropriate level of funding, their research would lead to working fusion reactors at any point from the year 2000 on according to the amount of funding their research received. Since then, funding for fusion research has dwindled considerably, forcing researchers to push back the date at which they expect commercial reactors to make their debut. In the interim, however, they have learned a great deal more about the science and technology of fusion reactors.

“DOE has an energy and a science mission,” explains Batchelor. “We’re in the uncomfortable position of being in both. Until about five years ago, fusion appeared as an account called energy. Then we were moved to the science account. Our research is definitely a science program, but it’s driven by an energy goal.”

It’s also driven by success. Last year the stellarator design team won ORNL’s award as research team of the year. Continued success seems guaranteed as the team builds their stellarator that will point the way to a working fusion reactor.
Detecting Defects

WHEN SOMETHING YOU’VE PURCHASED IS DEFECTIVE, you usually send it back for a replacement, or throw it out and buy a new one. If you happen to be in the explosives business, however, the opposite holds true, for when it comes to creating explosions, defects are a good thing. In fact, detonation cannot take place without them.

But, as with virtually everything else in life, moderation is the key to desirable defects. Too many defects make an explosive material unstable, and therefore unsafe, while if there are too few, it won’t detonate at all. But with just the right number of defects, the material will explode precisely when it is supposed to, and under just the right circumstances.

The defects in question are pockets, or voids, within and between the grains of chemical explosive materials. Once such a material starts to explode, the resulting pressure attempts to fill in those voids. As the material changes shape to flow in and around the defects, it becomes hotter than material away from them. The process of heating by changing shape also occurs when one bends a paper clip back and forth. The work of flexing releases heat.

In the case of explosives, as the voids are filled in and the nearby material becomes hotter, chemical reactions begin to occur at a faster pace. If the hot spots are big enough and hot enough, the organic molecules in the explosive begin to decompose, forming hot gas, and boom! An explosion takes place.

But determining the optimum number of defects to build into explosives is no easy task. Trial and error has been the answer to date. But, of course, when it comes to explosives, error can be especially undesirable. So it was to take the guesswork out of the equation, by bringing the precision of computational science methodology to the task, that the Grain-Scale Dynamics in Explosives (GSDE) project was created at Lawrence Livermore National Laboratory (LLNL), Livermore, California.

“Because we are trying to do is harness the power of the Advanced Simulation and Computing Initiative (ASCI) at Lawrence Livermore to computationally look in detail at the behavior of explosives to help guide their design,” says Jack Reaugh, who heads the project.

Under ASCI, a set of supercomputers has been created by tying together thousands of central processing units (CPUs) into one “massively parallel” machine. Complex problems are divided up among the CPUs, each of which solves some of the equations, thereby greatly speeding up the computing process. “The achievement of these machines is not so much that each CPU is much faster than any other, but that there are so many of them harnessed together,” explains Reaugh. As a result, when it comes to supercomputers, the ASCI system “is as super as you get,” he says.

ASCI was created to advance the state of computing hardware and software for all of DOE, and Reaugh’s project is but one of many that make use of its computing capabilities. In fact, without ASCI it would be a practical impossibility to run the kinds of detailed computations necessary to analyze defects in explosives.

Nuclear Stoichiople Safety

The GSDE project has been under way for four years, and though Reaugh hopes to expand its research to cover other types of explosives in the future, for the moment the group is using its computational prowess to focus on keeping the nation’s nuclear stoichiople safe, since chemical explosives used in the nuclear firing sequence.

Safety is an issue for the chemical part of the stoichiople because these explosives are organic, and as such they can change over time. If the defects change, the explosives may become more or less sensitive than they were originally intended to be. The goal of the computational group is to be able to predict whether such changes impact the effectiveness and safety of the explosives. “So far, we’ve accomplished some things, but we are not at the point of declaring victory,” says Reaugh.

One of the first hurdles the group surmounted involved developing a method of computationally describing the makeup of the plastic-bonded explosives used in the stoichiople. These explosives are produced by using a plastic binder to coat the grains, or crystals, comprising the material and then compressing them into a high-density mass. So that the grains fit together during the compression
process, they must be of widely varying sizes. This allows the smaller plastic particles to coat pieces to fit into the larger pieces between the larger pieces.

Creating a computational mesh that accurately accounts for the particle size distribution is an extremely difficult task. And, “if you don’t get the particle size distribution right, you don’t get the distribution of the defects right,” notes Reaugh. Although the researchers have succeeded in developing a realistic computational model of particle size distribution, some of their ongoing tasks is to refine even further for better mathematical approximations.

**Microscopic Tricks**

To derive the information from which they create computer models of explosives, the researchers borrow from empirical experiments and from their knowledge of basic physics. One way of deriving empirical information is “to use certain tricks of microscopy to look at crystals that go into the formation of these explosives and visualize what the defects look like within each of the particles,” says Reaugh. But microscopes are not of much help when information is needed about what actually happens in an explosive shockwave as the defects collapse and additional heat is released.

“One of the keys to knowing the extent to which an explosive will begin to detonate under a shock pressure is knowing something about the speed of the defects and their direction,” says Reaugh. But, he adds, “That was not known because it is difficult to perform experiments at pressures of a few hundred thousand atmospheres.”

Yet such difficulty did not dissuade another group of LLNL scientists, whose help he enlisted to perform the high-pressure experiments. To do so, they use a laboratory apparatus known as a diamond anvil cell. It includes two opposing diamonds, each about one-half of a millimeter in size, separated by a gasket containing a small sample of material under test. The strength of the diamonds keeps the high pressure contained as a laser melts the material, and the resulting deflagration is recorded on high-speed film.

A related example of cross-pollination is found in the development of the software that Reaugh’s group is using: “A cast of about 30, who are independent of my project, are developing physics and chemistry models and the numerical methods needed to solve the models in the computer simulation program that we use,” says Reaugh.

The program they develop is dubbed ALE 3D, with the ALE standing for Arbitrary Lagrangian Eulerian — Lagrange being a French mathematician and Euler a Swiss mathematician. The hydrodynamic equations used in the program make use of two frames of reference, each associated with one of the mathematicians. The Lagrange frame provides a mathematical mesh that, in the simulation, moves with the explosive material. “It’s as though a mesh is painted on the material, and as it moves about the mesh moves with it. The alternative is a Eulerian frame where the mesh is fixed in space and the material flows through it,” explains Reaugh, a physicist himself.

By making use of this general software tool, which is available to many researchers using the ALEI computers, “hydrodynamic flow, heat transfer, and chemical reactions were already recorded on high-speed film. “We could, in principle, do the calculation for a large piece of explosive,” he explains, “but it would require so much memory and so long a computational time that with the tools we have now,” he adds.

“Doing these calculations we use models to describe the behavior of materials, which are, by their nature, approximate. In some cases they were accurate, and in some cases they weren’t, so revising the models, describing the materials better, and looking in more detail at what the defect population really is, are all factors that can be examined computationally with the tools we have now.”

Current planning calls for the GSDE project to continue its work for at least four more years. And when its goals are fully and satisfactorily accomplished, it will undoubtedly go on its way, albeit one that will contain no surprises.

Which does not mean that the GSDE project’s work is stymied. On the contrary, “We have plenty to do,” says Reaugh. “We went through the process for the first time, and like anything you do for the first time, you learn how you should have done it, and what you should have done better.”

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Calculating Quarks

PARTICLE PHYSICIST DR. ROBERT (BOB) MAWHINNEY paints a picture of the subatomic world that makes you want to hit the replay button. It's dizzying. You lean closer, squint, as he describes his specialty, quantum chromodynamics (QCD), the study of the interactions among particles that have color charge—quarks and gluons.

OK. Quarks aren't that foreign. The six flavors of quarks are the bare-bones constituents of all matter. We are mostly quarks. Combine two up-quarks and a down-quark and you have a proton. As for color charge (hence the 'chromo' part of QCD) it's the quark-gluon equivalent of the electric charge in electromagnetism. Just as electrically charged particles interact by exchanging photons, in strong nuclear interactions color-charged particles interact by exchanging gluons.

When it gets messy, even for QCD devotees, is when you try to calculate the interactions between quarks and gluons. Sure, at high energies this world of strong quantum fluctuations is quite linear. It's at low energies, at the level of the proton, that things get messy. A quark turns into a quark plus a gluon. Then it interacts with another quark via a second gluon, while the first gluon turns into a quark/antiquark pair, then back to a gluon, and is reshuffled by the first quark. "You just have this enormously complicated, wavelike nonlinear sea of virtual particles. It's a perfectly poised computational problem," says Dr. Mawhinney, a professor of theoretical physics at Columbia University. "We have great faith in the underlying QCD equations because they're built on the principles of relativity and quantum mechanics, and at high energies, where we can calculate analytically, the results agree with experiment. But there are many phenomena predicted by the equations that we couldn't calculate with pencil and paper. So, it comes down to a question of computational strength to be able to calculate the physical consequences."

To do this, Mawhinney is part of a team from Columbia, the RIKEN Brookhaven Research Center (RBRC) at Brookhaven National Laboratory (BNL) and IBM that is designing and building the latest in a series of massively parallel computers to numerically probe the world of QCD. The 16-Tflops peak performance supercomputer, dubbed "QCD On a Chip," (QCDOC) is set to be booted-up at BNL in early 2004. QCDOC won't just push the bounds of quark-gluon physics—including understanding of the universe's early evolution—it's also a world-leading demonstration of the power and promise of topical computing.

Custom Made, Please

"There are only a few machines in the world that are built specifically for a topic," says Ed McFadden, who manages Brookhaven's Scientific Computing Facility, where QCDOC will be housed. But the 40-year BNL veteran (whose first computational problem had nothing to do with quarks, but rather with solving the four-color map problem) notes that these purebred machines are attracting more interest than ever, including the interest of DOE's SciDAC (Scientific Discovery through Advanced Computing) program, which is demonstrating the power and promise of topical computing. QCDOC will be the latest iteration of a computational vision first adopted by Dr. Norman Christ in the early 1980s. Since that time, the now senior Columbia physicist has been leading the design of QCD-specific computers. When Dr. Mawhinney arrived at Columbia as a post-doc in 1990, Dr. Christ was modeling quarks and gluons on a custom-built 25-Mflops, 16-Gflops machine. Within a couple of years, the pair—along with Dr. Al Gara, now at IBM, and a team of graduate students and post-docs—had set their sights on greater things: a 1-Tflops, 20,000 processor massively parallel computer, the QCD on Digital Signal Processor (QCDSP). The first QCDSP, funded by DOE, came online at Columbia in early 1998, and a second one, funded by RBRC, at BNL later that year.

The QCDSP was the perfect computational fit for the experimental work being done in BNL's Relativistic Heavy Ion Collider (RHIC).

"One of RHIC's primary goals is to detect a quark-gluon plasma, a phase of matter thought to exist in the early universe, in which quarks and gluons aren't bound into protons but are a gas or plasma. It's a very tricky thing to do experimentally, and nobody's been able to convincingly detect it yet. However, in the QCDSP we can calculate the properties of this quark-gluon plasma state, such as temperature and pressure, which can feed into the theoretical predictions for RHIC physics and our understanding of the early universe," says Dr. Mawhinney.

Still, why the years of time and effort to build a custom machine? "Cost," says Dr. Mawhinney without a pause. He estimates that the approximately $4 million to build the QCDSP was about one-tenth the price tag of an equivalent commercial massively parallel machine at the time. But for Mawhinney and the rest of the QCDSP and QCDOC team, the benefits of a dedicated machine extend far beyond the initial cost savings. These machines represent the chance to optimize the hardware and software to your science. In this case, the result has been the creation of compact, low-operating-cost machines of enormous reliability. (See sidebar Small is Beautiful on page 33).

QCDOC won't just push the bounds of quark-gluon physics—including understanding of the universe's early evolution—it's also a world-leading demonstration of the power and promise of topical computing.
Science on a Grid

The point of departure for the optimization of these QCD machines is lattice gauge theory. The theory enables the calculation of quantitative QCD equations by drawing up space and time into a regular grid of points. “It’s a critical step in how we take the equations and map them into the computer,” says Dr. Mawhinney.

What the QCDSP and QCDOC teams have done is to configure the computational architecture specifically for these grid-based lattice QCD calculations. With both machines, the processors are organized in a regular grid, four-dimensional for the QCDSP and two-dimensional for the QCDOC. Each processor handles all of the variables for one local volume of space-time. This design optimizes nearest neighbor communication, the critical issue in QCD since the forces between neighboring points are local.

QCDSP and QCDOC use a simple mesh in the hardware. So, we’re able to achieve very low latency for the communication between these neighboring nodes. This allows us to get very good efficiency.” It also means that these machines are able to apply a large number of processors to a fixed size problem. “This is one of the most difficult kinds of scaling for a parallel computer,” notes Machinney.

He stresses that the software components are as important as the hardware. “The advantage of targeting QCD is not only that it’s the first application in terms of the hardware, but also that we have a whole range of things to handle with our software,” Machinney says. As a result, the custom operating system is “lean and small,” with little code, in order to minimize the software overhead.

The project is now also able to benefit from in-age: the physics software written for the QCDSP in C++ will be migrated to QCDOC.

Gen-Next Hardware and Science

QCDSP’s design is benefiting both from the experience gained with QCDSP and the telegram, now international, lattice QCD computational collaboration. Two QCDSPs are presently being built, one at BNL and the second 10-Tflops machine for the United Kingdom QCD group based at the University of Edinburgh. In addition to DOE and RREC support, this UK-UK partnership has funded money into the design project. The international collaboration also added manpower, primarily in the form of Dr. Peter Boyle, a post-doc from the University of Edinburgh who is based at Columbia, and Dr. Tilo Weing, a Yale physics professor, who has a joint appointment at BNL.

With $5 million in funding from RREC, the University of Physical and Chemical Research in Japan to complete the project in 2005. QCDDOC will compete in the third mainiona faster processor, more local memory, and faster nearest neighbor communication.

QCDDOC’s 10,000 nodes, each of which will be 20 times faster than those on the QCDSP, will be designed based on an IBM Power 4 440 ASIC template. The primary reason for this choice is that such a design has been led by the Columbia team in collaboration with Dr. Gara — will have 4 Mbytes of memory on the silicon wafer and a high-speed interprocessor network designed by Dr. Gara and collaborators at IBM.

The additional increase in performance QCDSP’s, plus 10-Tflops peak performance, is needed for other more memory-intensive theoretical physics grid-based applications, a possibility that’s now being considered in terms of broadening the machine’s use.

The increased computing power QCDDOC will provide is just what Dr. Mawhinney and others need to clear the QCD fog of non-linearity. To date, he says, researchers have used an approximation, called the quenched truncation, to navigate around a key part of this non-linearity in the calculations. The real qualitative step that everyone is looking for so we go from a L-Tflops machine to a 10-Tflops one is to remove this approximation so that we will actually be handling all the non-linearity,” says Dr. Machinney. QCDDOC will allow the improved study of quarks even in a bound state as color-neutral hadrons.

However, the impact of these custom machines is extending beyond QCD science, into parallel processing throughout the high performance computing community.

“Many other high performance users are extremely impressed with QCDSP,” says BLN’s McFadden. “But on the other hand, we get into this whole Blue Gene/L parallel machine, and then we’re thinking about how QCDDOC, in terms of developing the hardware, and then writing the operating systems are maintaining this whole thing. That scares the hell out of a lot of people, and think the success with QCDSP will have people giving it a second look, especially in terms of cost.”

Indeed, the QCDOC-computing program has already had a notable computational spinoff: IBM’s planned Blue Gene/L supercomputer. This 360-Tflops peak performance machine’s main hardware architect is Dr. Gara of QCDSP and QCDOC fame. Bound for DOE’s Lawrence Livermore National Laboratory in 2015, Blue Gene/L represents an extension of the grid-based application hardware-structure pioneered in the QCD machines.

While others watch and assess the performance of these QCD machines, for Machinney the excitement over the design of a new machine is mounting into the expectation of what it will help tell us about the world of quantum chromodynamics.

“There is a tremendous advantage to being able to put theory and experiment to the test, and QCDDOC will enable us, ever more accurately, to test our theories against the experiments. And where the discrepancies will show up, where we’ll see the next hint of new physics, you don’t really know. But it’s the tool that lets you ask the questions.”

SMALL IS BEAUTIFUL

This diminutive size has broad repercussions — in terms of cost, performance and reliability — for the quantum-chromodynamics science that QCDDOC will perform.

QCDOC’s designers chose to use processors of mid-range speed, thereby optimizing overall performance and drastically reducing the energy consumption and heat output per node. Each QCDOC node will use less than two watts, allowing the nodes to be tightly packed in this water-cooled machine, and making 80% more energy efficient than Japan’s Earth Simulator.

“The science is very directly impacted by the low electrical power, and the small footprint of these machines,” says Columbia University particle physicist Dr. Robert (Bob) Mawhinney, one of QCDOC’s principal architects. “Because the electricity and the room to house the machine don’t cost as much, we can actually get enough computing power to really push the science ahead without sacrificing every post-doc, graduate student and travel grant in our entire budget.”

QCDDOC’s compact nature also means fewer components and cables, and thus less chance of mechanical breakdown. This is already the case with QCDSP’s predecessor, QCISP.

“One of the most impressive things about QCISP, and we expect about QCDDOC, is that it is less than 0.73% carbon dioxide in the past three years,” says McFadden. “It’s extremely reliable.”
In 1994, nuclear engineer Doug Kothe requested internal research funds from the Los Alamos National Laboratory for a small scientific project. His objective was simple. He wanted to extend to three dimensions a two-dimensional computer model of free surface flow — the changing interface between liquids, such as liquid helium and water, and gases, such as air, as they flowed past each other — that he had completed for the National Aeronautics and Space Administration. With financing from Los Alamos’s Laboratory Directed Research and Development (LDRD) project, Kothe not only applied his computing code to an extra dimension; he also broadened it so that it could be used to model free surface flow between any gas and liquid.

Since then, the project has blossomed far beyond the single-scientist study that Kothe envisioned. Called Telluride, it helps to simulate the methods used for processing uranium, plutonium, and other metals critical to the country’s stockpile of nuclear weapons. “The overall aim is to provide computer simulation of materials processing for the nuclear weapons complex,” explains Telluride’s present project leader Jan Sicilian. As an indication of Telluride’s importance, responsibility for financing it has moved from LDRD to the National Nuclear Security Agency’s Advanced Simulation and Computing (ASC) program, a project that spends $700 million each year to give government scientists and engineers the technical capabilities they need to maintain a credible nuclear deterrent without underground nuclear testing.

Telluride has potential applications beyond simulating the processing of nuclear materials. “We collaborate with universities and other government labs to develop new models,” says Sicilian. “We provide source code and exchange scientists with them, and we often have graduate students and postdoctoral fellows come to study with us. And some outside researchers have developed extensions of our work to apply to their own problems that we might ourselves pick up for the future. We have about a dozen collaborative agreements of that type.”

Opportunity for Application

The creation of ASC in 1996 provided the opportunity to apply Kothe’s original project to real and significant security needs. As it happened, Los Alamos had recently taken over the task of processing metals such as plutonium and uranium into parts for nuclear weapons, a task previously performed by a Department of Energy facility in Rocky Flats, Colorado. “My group leader, John Hopson, told me that my code could be used to model mold filling for our foundries,” Kothe recalls. “Surprisingly, liquid metals behave much like water.”

Hopson did more than determine the vision for Kothe’s untitled project. He decided that it would benefit from having a name. “As an avid skier, he named it after Telluride, Colorado,” says Kothe. “We tend to name Los Alamos projects after southwestern geographies.” Following that example, the team later gave the name Truchas — Spanish for trout, and the name of a peak in the Sangre de Cristo mountain chain in New Mexico — to the first Telluride software that it released outside the Los Alamos National Laboratory. “The idea of using simulation processing has about 20 years of history behind it,” Sicilian himself devoted 15 years to seeking for a small company developing a commercial program for metal casting analysis. “The Telluride project continues to give government scientists and engineers the technical capabilities they need to maintain a credible nuclear deterrent without underground nuclear testing.”

Sicilian says, “No commercial products have all the features we need for simulation of our processes. That’s the reason Telluride exists.”

Simulation offers obvious advantages in the development of methods for processing difficult-to-handle metals such as plutonium and uranium. “It’s a lot cheaper and faster to do it computationally rather than carry out the real thing, especially as the materials are expensive and dangerous,” says Sicilian. “The payoff in the weapons projects is larger than it is in other areas because the experiments are exceedingly costly and time-consuming. To meet timelines by doing many experiments is not an acceptable approach.”

Computer simulation offers model producers a more fundamental advantage: “We can learn things that experimenters are unable to measure without disturbing the system,” Sicilian continues. “For example, when people here do experiments, they measure the temperatures in the mold material, not in the metal itself. Recent simulations of ours have shown that there can be significant differences depending on the thermal history of the metal.”

Two Problems

Almost as soon as he agreed to the concept of applying his research to real-life metal processing, Kothe realized that he faced two problems. “First,” he says, “engineers at our two foundries — one for plutonium and the other for other metals — hadn’t asked for models. And as a nuclear engineer by training and a computational fluid dynamics by practice, I had no idea of the complexity of the physics involved.”

The complexity stems in part from the fact that the free surface flow characteristics involved in processing liquid metal into a mold cast are represent only one component of the processing that needs to be modeled. Even before the liquid metal is poured into the mold, the software
must predict the distribution of temperature in the mold material induced by electromagnetic heating. Also, the alloy cools and solidifies in the mold. Further cooling of the solid metal to room temperature completes the casting process. Next, the alloy part undergoes further heat treatment to homogenize it. Finally, machining prepares the part for integration into the system for which it is designed. This sequence of events means that Telluride must provide realistic models for solidification of the alloy, in other words, for the large segregation effects involving alloy components, free surface incompressible flow, heat transfer, complex three-dimensional geometric effects, microstructural modification and evolution, solid state transition effects, and the residual build-up of stress and strain that develops in response to those effects. So while the application of Telluride to the initial goal of helping foundry workers to understand and optimize their casting processes, it should also facilitate the design of new casting processes for alloy components that possess specific properties in the micro-scale. Our overall aim is to predict the properties of the metal alloy itself, to help improve casting settings and to optimize the system for which it is designed.

Furthermore, Telluride’s team started by comparing experimental reality with Telluride simulations of water poured into a plastic mold. Having satisfied themselves that the software accurately predicted reality, team members then used it to predict the cooling rate and expected grain size of real metallic foams. That work resulted in two critical objectives: it validated the software and it validated Telluride’s capability to model real events in metal and alloy processing by checking its predictions against experimental findings.

Once the foundry teams showed the benefits that Telluride modeling could provide, the Los Alamos team realized that the approach could help them. In 1999, the group responsible for welding transuranic metals and their alloys approached the Telluride team for assistance. Kothe says, “tellurium is not something we had been working on before.” Kothe explains that the group was involved in developing the foam parts used to contain component parts in the complex structures of nuclear weapons designed for the U.S. As “in-house” developers, they could not afford to model chemical reactions that occur during the curing process for the foam. The next step was the transformation of the foam from a wet material to a dry material in the baking oven.

Computers and Collaborations

One of the beauties of Telluride’s software is its ability to run on a broad range of computers. Kothe recalls that while working on the program a very wide variety of platforms, from personal computers to the latest supercomputers at Los Alamos, Sicilian points out. “Ultimate scalability is one of the project’s goals and it will benefit from the computing power available at Los Alamos. Thus far we’ve never really been able to do development and testing work on fairly easily available machines,” he continues. “But once we get into really serious calculations, we’ll move up to two orders of magnitude to the big ASCI computers, a group that are unique in the world.”

Los Alamos offers the Telluride team another benefit: the variety and quality of its scientists. “The great thing about working for us because it has so many people with diverse backgrounds,” says Kothe. “We had physicists, computational scientists, engineers, computer scientists, and other collaborators with us. We’ve had regular informal contact with the experimentalists. A large research institution is the only place at which something like this can be done. Telluride is a national lab atmosphere.”

As a result of that experience, Kothe possessed the necessary intellectual breadth to lead the Telluride project when it expanded from his original idea. He continued his role when he was promoted to the middle management position of group leader in October 2002, but left Los Alamos in October 2003 after two years. Nevertheless, he remains an active member of the Telluride team, spending time on technical details of fluid flow algorithms and models.

Plutonium and Uranium

Hopson and Kothe expected that Telluride would prove its value for plutonium processing first. After all, Kothe says, “plutonium is not something I had been working on before.” Kothe explained that Plutonium-239, a radionuclide, was developed in response to those effects, and the residual build-up of stress and strain that develops in response to those effects. So while the application of Telluride...
STOMPing Ground

**IF YOU LIKE A GOOD MISNOMER**, you need look no further than the Scenic Highway site outside Baton Rouge, Louisiana. There, spread over 17 acres of graded dirt, are dozens of recovery wells. Down the road a mile and a half, at a place called Brooklawn, are more wells on 60 acres — 165 wells at the two sites, about a mile from the Mississippi River. Take in the view, but don’t drink the water.

Scenic and Brooklawn comprise the EPA’s Petro Processors Superfund Site where, in the 1960s and ’70s, for 13 and 11 years respectively, a “disposal company used to pour organic waste from petroleum companies into large ponds and trenches,” says Mark White, senior research engineer at the Department of Energy’s Pacific Northwest National Laboratory.

White is code author and custodian of STOMP, which stands for “subsurface transport over multiple phases.” STOMP parcels up a piece of ground into three-dimensional cubes, then simulates underground flow and transport of very bad things, environmental nightmares both happening and waiting to happen. White and his STOMP team at PNNL’s Hydrology Group try to get on the case before the nightmare has happened; their intervention can lead to action that can prevent a given pollutant from reaching groundwater.

At Scenic and Brooklawn, the nightmare was happening. A site-restoration company had cleaned up the surface, but as common sense might dictate, company had cleaned up the surface was happening. A site-restoration pollutant from reaching groundwater. At Scenic and Brooklawn, the nightmare was happening. A site-restoration company had cleaned up the surface and, as common sense might dictate, drilled wells from which to pump out the nasty stuff that had seeped downward. White’s word for that stuff sounds like ‘Drain Apples’ — DNAPLs, dense-nature-water nonaqueous (oily) phase liquids (NAPL), among the many forms of pollutants covered in the transport equations of STOMP.

In this context, the important thing about a DNAPL is that it sinks in water. Mark Ostrem, a senior research engineer in White’s group, ran a STOMP simulation for Scenic only to discover that the army of pumps, which had cost a small fortune to install and to operate and were intended to suspend the organic pollutants, actually made things worse. The model, also applied for Brooklawn, showed “that as millions of gallons of water flowed upward, the water table dropped,” White says. “The DNAPLs migrated farther down into the system and toward the drinking-water aquifer. They shut down the perimeter wells.”

As a result, recovered groundwater continues to be treated to remove hazardous liquids and other contaminants. Unlike its namesake, the Scenic simulation, and others, turn out to be rather elegant. STOMP solves a series of equations that describe the physical properties in the hydrology system under investigation. The program can be tailored to track the migration of materials through water, brine, ice, oily liquid pollutants, through just about any fluids that might fill underground pores, thanks to a called variable source code that enables anyone using it to dial in the desired governing equations to be solved: water mass, air mass, dissolved-mass, salt mass and heat. Equations-solve problems specific to transport of chemicals in solution, radionuclides decay and chemical reactions. At the end of this process is a time-lapse picture of underground plumes of pollutants expanding and receding, depending on how the intrusive chemicals interact with the soils and elements in the ground, under any conditions the modeler can conceive of.

“We have put the simulator through a rigorous verification procedure against analytical solutions, laboratory experiments and field demonstrations,” White says. “I want to emphasize that the nature of this work is collaborative. Matt and I ponder why the numerical simulations don’t agree with the experimental observations. Numerical simulation solves a collection of mathematical equations in an attempt to describe physical processes.

Typically these equations do not completely describe the modeled systems, as assumptions were taken or processes were ignored to generate the equation sets. This is where the art of numerical modeling comes in — deciding how to mathematically describe observed multifluid flow processes, and deciding which equations to include in the collection. If one...
Simulated CHAP saturation at year 2080 for the Site Operable Unit near Baton Rouge, LA.

COLLABORATORS

**Mark White** is the principal author of STOMP and is a Senior Research Engineer in the Hydrology Group at Environmental Technology Division at Pacific Northwest National Laboratory (PNNL). He has been at PNNL since 1986 and his current research interests include developing mathematical descriptions of experimentally observed multi-phase fluid flow and transport processes and applying these descriptions to the effective modeling of contaminated subsurface environments through field-scale technology development or deployment. He received his BS in physics from Pennsylvania State University, and his MS and PhD in mechanical engineering from Colorado State University.

**Mart Oostrom** is a Senior Research Engineer in the Hydrology Group/Environmental Technology Division of Pacific Northwest National Laboratory (PNNL), where he is responsible for projects related to multi-phase fluid flow and transport model development. Current projects include the development of a theory for relative permeability hysteresis in sandstone. He has worked in remote-sensing and porous media, the investigation of surfactant-enhanced aquifer remediation techniques for clean-up of aquifers contaminated with chlorinated solvents, and the development of algorithms for fluid and transport. A native of The Netherlands, Dr. Oostrom received both his BS (solid science and geology) and MS (soil physics) from the Wageningen Agricultural University in The Netherlands. He received his PhD in soil physics from Auburn University.

Further Reading: For more information on STOMP, White, Oostrom and their team, please see their Website at: [http://www.pnl.gov/stomp](http://www.pnl.gov/stomp)

**Contact:**

**Mark White**

mark.white@pnl.gov

**Mart Oostrom**

mart.oostrom@pnl.gov

PRACTICUM COORDINATOR

Janet Jones-Oliveira

jeolie@pnl.gov

STOMP author Mark White and collaborator Mart Oostrom are part of the Hydrology Group in the Environmental Technology Division of Pacific Northwest National Laboratory. White says that while each national lab has a program for modeling the subsurface, PNNL has a mandate to give those capabilities macho-sounding acronyms like STOMP. Lawrence Livermore has its NUFT, and, not to be outdone, Lawrence Berkeley has TOUGH.

By no means a new or even objective measurement, STOMP would have to be ranked among the top of these contenders as one of the most widely tested systems. The technology—Biocore, the nonprofit corporation that operates PNNL and other national labs, feels its copyright to the code—has transferred well. Besides the national labs and government agencies, STOMP has been invited by private companies and universities alike and has been run on a great variety of hardware, ranging from personal workstations to Beowulf clusters and supercomputers around the world.

White, a mechanical engineer by training, continues to adapt the STOMP code to new applications and to ramp up its performance. STOMP’s impact and successes are well documented in the professional literature, as well as in more accessible places. While his professional framework is spelt out in a theory guide available on the Web, along with an application guide and a user’s guide. Oostrom, whose background is in physics, is co-author of the guides and keeps the code itself, checking it against experimental results.
LITTLE DID PAUL FISCHER KNOW that a convivial hallway chat outside his office at Argonne National Laboratory would lead him on a “fantastic voyage” into the turbulent world of an artery on the verge of causing a stroke. Like the characters in the 1966 sci-fi film classic, a team of scientists has ventured into the bloodstream to see what happens inside a blocked artery. But this voyage is a virtual trip, combining computational prowess with advanced medical imaging and fluid dynamics — all with an eye to preventing a devastating stroke.

It was in the summer of 1998 that Fischer struck up what he calls a “serendipitous conversation” with visiting scientist Frank Loth, a specialist in fluid mechanics from the University of Illinois at Chicago. Loth was working on computer simulations of blood flow inside arteries. The two began to chat about the challenges of modeling blood flow, particularly when blood rounds a bend in an artery where mechanical forces can cause tiny eddies and whirlpools to form. “Frank mentioned that he had a couple of cases where the blood flow transitioned to turbulence and I said ‘We can do that,’” recalls Fischer. It turned out that Fischer specializes in creating computer programs that model turbulent flow in complex domains, just what Loth needed to understand the effects of turbulent behavior on the formation of potentially deadly atherosclerotic plaque.

Tying to understand the physical forces that govern blood flow, new scientists have been publishing treatises on the subject for decades. But only in the past few years has a confluence of technologies made it possible to create a realistic and useful computer model of turbulent blood flow.

Even the equations that Fischer uses to describe fluid flow have been in use since the nineteenth century. But only in the past few years has a confluence of technologies made it possible to create a realistic and useful computer model of turbulent blood flow. "We want to understand what is particular about one person that causes atherothrombosis disease versus other people who don't have disease," says Fischer. "It turns out that geometry is very important in determining null shear stress, which is the action of blood on vessel wall. Now we want to learn, is it the shape of the vessel? Is it the flow conditions? What are the important factors in formation and stability of plaque?"

Loth and his longtime collaborator at the University of Chicago, Hisham Bassioni, a vascular surgeon, are specifically interested in the carotid artery, the main artery that supplies blood to the brain. It turns out that the carotid is a prime location for fatty plaque to build up, narrowing the vessel diameter and forcing the heart to work harder to get blood into the brain. Over time, this plaque buildup can become unstable. When small pieces break off, they travel to the brain and can become lodged in smaller vessels. Blocking blood flow and causing brain cells to be starved for oxygen so that they die within minutes. The phenomenon is so common that since you started reading this article someone in the U.S. has had a stroke.

The Chicago-based scientists began the collaboration with Fischer with one question in mind. Who is most at risk for a stroke? And particularly, who is most likely to lead to stroke? Being able to predict with some certainty who is at greater risk would help tremendously in deciding who should undergo carotid endarterectomy, an operation in which surgeons split open the carotid artery to remove potentially deadly atherosclerotic plaque. In addition, says Fischer, the simulations could help determine if grafted arteries and veins are prone to failure due to mechanical forces.

"Frank Loth is really the driver of the science behind this project," says Fischer. "As a biomedical engineer, he understands the biology and he understands the fluid mechanics. He really holds it all together."

But to create realistic models they needed some way to model turbulent conditions inside the carotid. And it isn’t enough to do the calculations on an idealized approximation of an artery, because each person’s carotid artery is a different shape, changing dramatically the conditions inside the vessel walls.

To develop a realistic simulation, the team first had to develop a way to convert data collected from medical imaging devices such as a CT (computed tomography) or MRI (Magnetic Resonance Imaging) scan into a three-dimensional representation of the vessel wall. Seung Lee, who at the time was a student at the University of Illinois at Chicago, spearheaded that part of the project. Lee, now a graduate student at MIT and a DOE CSGF fellow, developed software to convert two-dimensional slice-based data into a three-dimensional mesh described by grid points and organized computationally into “bricks.” Within each brick the physical forces of velocity and pressure are described mathematically in terms of a polynomial function.

The conditions inside the vessel walls at any point are described by the number of grid points required,” says Fischer. The reason is that in a smooth laminar flow the force is mostly uniform and in one direction, as you see in water running from a faucet that is turned on slightly. But in turbulent flow, the force is constantly changing, and the number of grid points required is constantly changing as well.

At this point, Fischer and his Argonne colleague Henry Tufo entered the picture, providing the computational means to describe the turbulent flow: "All the vortices associated with turbulence dramatically increase the number of grid points required,” says Fischer. The reason is that in a smooth laminar flow the force is mostly uniform and in one direction, as you see in water running from a faucet that is turned on slightly.
If you suddenly turn the faucet on full force, you get jets and bubbles. "Imagine trying to describe that computationally and you get some idea what we are trying to do," he says.

"And on the time scale," he adds, "if we want to model the force exerted during one heart beat we suddenly go from needing a minimum of 30 time points per heartbeat to thousands of time points per heartbeat."

The behavior of blood flowing inside a vessel is governed by the Navier-Stokes equations. It is relatively easy to model smooth, laminar blood flow, and in fact there are probably at least 30 laboratories worldwide that are doing so, says Fischer. But when you introduce turbulence into the equation, the level of computational complexity increases tremendously.

To make the calculation possible, the team employs a computational tool called the spectral element method, which allows them to divide the calculation into discrete computational blocks that are ideal for numerically solving the Navier-Stokes equations on a massively parallel computer system. The spectral element method, explains Fischer, also excels at calculating flows that are just near the onset of turbulence, as is the case for blood flow.

Once the team had put all the elements in place it was time to put their algorithm to the test, to enter the world of a blocked artery and see what is happening inside. With Bassiouny providing real-world imagery data of a patient whose artery was severely blocked, the team ran their algorithm on Pittsburgh Supercomputing Center’s Terascale System, which has a storage capacity of 100,000 times that of most desktop PCs and a thousand times the computational capability. The goal: to arrive at a realistic simulation within 24 hours, quickly enough to generate data in a time frame where it can eventually be used to help direct clinical decisions.

The first simulation, done in mid-2000, passed with flying colors. Loth’s group continues to conduct controlled experiments to compare to the simulations to provide quality control, and the agreement between the numerical and experimental models has been impressive.

From the computational standpoint, the algorithm can now calculate a single cardiac cycle in 10-20 hours of CPU time on 256 processors. In fact, so promising that the team has stepped up efforts to push the process even further.

In order to have efficient iterative methods for systems involving millions of gridpoints, you need to have multilevel algorithms that can quickly improve the solution at the fine and coarse scales. To scale this approach to hundreds of processors, it is important to have a fast coarsegrid solver, since that’s typically a communication intensive process. “One of the things we’ve done is develop a very fast parallel coarsegrid solver, but we are trying to further improve the speed of the overall process by introducing additional intermediate grids, which will result in a multigrid algorithm,” says Fischer.

For vascular surgeons like Bassiouny, the real payoff will come when it is possible to gather real-time data from medical imaging devices and feed the information directly into the modeling software. At that point, it would be possible to conduct a series of clinical trials in which the computer simulations are correlated to patient outcomes and it becomes feasible to predict who is most at risk for stroke.

“‘One experience,’ explains Bassiouny, ‘is that many people can live for years with fairly extensive plaque and never have a stroke, while someone else may have less plaque, but if it’s unstable the risk is much greater.’

Fischer emphasizes that in addition to its medical applications, the algorithm can be used for studying heat diffusion and other types of fluid flow, whether liquid or gas.

“We have a dozen groups around the world using the code for different applications,” says Fischer. ‘The Nek5000 code provides researchers with direct access to advanced parallel algorithms.’

In the words of Dr. Peter Dural, the surgeon in Turin, “We stand in the middle of a fantastic voyage of knowledge.”
Tom Epperly

IN THE BIBLICAL STORY OF BABEL, people become disorganized and scatter across the land when they suddenly find everyone around them is speaking a foreign language. They surely could have used a guy like Tom Epperly.

As a project leader of the components group at Lawrence Livermore National Laboratory, Epperly creates code that allows computer languages to talk to one another. The group is part of a larger multiinstitutional partnership called the Common Component Architecture Forum that is developing component technology for scientific computing.

“The main thing we are after here is code reuse,” says Epperly. “We are providing technology that enables people to reuse other people’s work, and in the process we are saving money and making sure the ‘best in class’ solutions end up in other people’s hands.”

The goal of component technology, says Epperly, is to create a software library that allows programmers to pick and choose the applications best suited for their problem and then allows all the components to work together seamlessly. Component technology, says Epperly, is what makes it possible for users of Microsoft products to cut and paste an Excel spreadsheet into a Word document and then put the whole thing into a FrontPage Web site.

Of course, the programmers at Microsoft had interoperability in mind when they wrote their code. Epperly’s job is much trickier, since he is working with languages created long before anyone envisioned today’s high performance computing environment.

“Fortran is still a major language in scientific computing,” says Epperly. “In contrast, the mainstream computer science world is dominated by languages such as Perl, Java, C++, and Visual Basic. My mission is to upgrade the state-of-the-art for software development in scientific computing.”

Today, he says, most programmers are developing code in an object-oriented programming style and his group adapts code to work with these programming styles.

Epperly’s main customers are programmers at the national labs and in academia who are developing high performance programs that run on large parallel computers. For example, his group developed a product they call “Babel,” that, appropriately, allows programmers to mix the languages C, C++, Fortran77, Fortran90, Java and Prolog in a single application. Scientists at Pacific Northwest National Laboratory (PNNL) are using Babel to allow various computational chemistry components to talk to each other during a molecular simulation.

Epperly started out as a chemical engineer, obtaining his PhD in 1995 at the University of Wisconsin at Madison. His postdoctoral work at Imperial College in London focused on design under uncertainty: how to build a chemical plant when demand for the product is unknown. His design optimized return on investment under conditions of uncertainty.

After a short stint working for a company that supplies software to the chemical industry, he decided to move on to new challenges.

“I wanted to be on the cutting edge of technology and the national lab presented a good balance of basic and applied research,” he says. “At the national lab there is an emphasis on research and application,” he says. “At the University of California Lawrence Livermore National Laboratory (LLNL), you have both, and both are considered valuable. The work I do here has an impact on real life decisions and situations.”

He says having a background in physical systems has helped him in his current work and has often made him an interpreter between the scientists and the computer programmers.

“It is important to understand the application area, which is modelling physical systems, in doing this work,” he says. “There’s often a gap between computer science types and the people who know the underlying physics. Having a joint background in engineering helps me bridge that gap.”

Tom Epperly says the goal of component technology is code reuse, “We are providing technology that enables people to reuse other people’s work, and in the process we are saving money and making sure the ‘best in class’ solutions end up in other people’s hands.”

Marc Serre

“Expert knowledge” is the title of a recent book by Marc Serre, assistant professor in the department of environmental sciences and engineering at the University of North Carolina at Chapel Hill.

Serre is trying to reconstruct the path of airborne pollution released by the collapse of the burning towers.

Marc Serre

IN THE AFTERMATH of the World Trade Center destruction many scientists mobilized to aid in understanding what happened. Engineers analyzed twisted girders. Forensic scientists helped identify victims. But as much of the initial frenzy of activity died down and the event itself recedes into history, Marc Serre’s work is just beginning.

Serre, an emerging expert in a specialty known as spatiotemporal geostatistics, is modeling the movement of toxic gases that emanated from the World Trade Center disaster site. Using a method he developed with former UNC mentor George Christakos, an expert in modeling of environmental systems, Serre is trying to reconstruct the path of airborne pollution released by the collapse of the burning towers.

“We have the best method to integrate all available knowledge,” says Serre, assistant professor in the department of environmental sciences and engineering at the University of North Carolina at Chapel Hill. “We have satellite data, weather information and expert knowledge. When you are able to combine all that, you have a better assessment of what people were exposed to after the World Trade Center collapse.”

Unlike previously used methods that could only model movement of toxic substances over space or over time, Serre’s method does both simultaneously, and is able to incorporate flow transport equations and so-called “fuzzy knowledge” or expert knowledge.

“This is a completely novel idea of how to incorporate that knowledge,” says Serre. “The framework we have developed is more rigorous and more flexible than the classical approach and we are able to incorporate all the knowledge bases to come up with a better assessment of exposure to toxic agents.”

“Professor Christakos had the idea for several years of using the Bayesian maximum entropy method to estimate the distribution across space and time of environmental agents,” he says. “It came at a very interesting point, where my background was just ideal to implement it. There was a kind of a spark. I provided the numerical implementation of his idea, and it all came together.”

Since the two developed this new way of tracking complex movement of substances during Serre’s graduate student days, the two have made the resulting program available on their Web site. Called BMElib (available for download at www.unc.edu/depts/case/BMELIB), the program can be used for a variety of applications. Serre himself has tracked the movement of things as diverse as arsenic in Bangladesh and sexually transmitted diseases in inner cities. He says his program is now in use worldwide to study things such as groundwater purity in Russia and the movement of bats in Spanish caves.

Serre’s current work focuses on improvement of the conceptual framework and the code performing the numerical calculation, which used to run mostly on high-end computers. However, the latest version can run on a PC, making it available to many more researchers.

“We have learned through our [DOE CSIG] fellowship is to combine mathematical sciences with smart high-level numerical implementation,” he says. “That’s exactly what we have done here.”

Marc Serre
Scott Zoldi

**COMPUTATIONAL SCIENCE** might not seem like the kind of training that would lead to a career as a private eye, but for Scott Zoldi a penchant for spotting changes in behavior has led to a career as a high-tech computational sleuth.

Zoldi’s training in computational and theoretical physics turned out to be just what they were looking for at a Fair Isaac Corporation, the largest U.S. company dedicated to detecting and reducing consumer fraud. As an analytic science manager, Zoldi leads a team that creates computer programs to analyze an enormous quantity of data and ferret out customers who are committing telecommunications fraud. This includes using call records to detect closed phones — actual physical copies of people’s cell phones that contain all information needed to make thousands of dollars of fraudulent calls in a very short time frame.

“One is so data-driven that one doesn’t understand what to do with it,” says Zoldi. “What you need is someone with a strong analytic and computational background to go and analyze call records and telerecords of information and reduce it down to predictable variables. What we do is separate out the good stuff and throw away a whole bunch of pulp.”

The goal is to help companies identify and define fraudulent behavior as quickly as possible.

“Since we operate in a business environment, we have to focus very much on return on investment,” says Zoldi. “We apply our computational physics training to create statistical models that mitigate fraud risk.”

Zoldi sees his current work as a direct extension of his graduate work.

“My research was kind of broad; it centered around complex problems with an abundance of data and looking for relationships in that information,” says Zoldi.

In graduate school at Duke University, Zoldi used his computational skills to create algorithms that helped doctors determine if antiepileptic medicine was working for the patient. The key was converting multiple brain scan readings into a useful pattern that could be computed before and after treatment.

Zoldi’s training in computational and theoretical physics has served him well at Fair Isaac, where efficient use of computational time is essential.

Within the company we have a large number of Unix and mainframe computers, and the computer builds machines from scratch specifically for training our neural networks,” says Zoldi. “We build our own analytic tools and computational algorithms because when we are processing huge volumes of data, and we have such tight deadlines, it’s really important that everything is done as efficiently as possible. If we write a bad code or don’t think very carefully about tuning our architecture to our program, it could take six years versus six weeks to solve a problem.”

Zoldi says he enjoys the challenge of working in industry.

“There is a lot of innovation here,” he says. “Our company employs well over 100 Ph.Ds in modeling. Personally, I find it a great challenge. It’s an environment where I can show the value and accuracy of my theories and my ideas. It is quite challenging and intellectually stimulating.”

“We apply our computational physics training to create statistical models that mitigate fraud risk.”

Howes Scholars

**THE FREDERICK A. HOWES SCHOLAR** in Computational Science award was established to honor the late Frederick Anthony Howes, who managed the Applied Mathematical Sciences Program in the U.S. Department of Energy during the 1990s. Dr. Howes was highly respected and admired for his energy, dedication and personal integrity.

2003 Scholars

Two candidates were selected as Howes Scholars in 2003. Dr. Jon Wilkening of Courant Institute of Mathematical Sciences and Dr. Oliver Fringer of Stanford University. Both Dr. Wilkening and Dr. Fringer were DOE CSGF fellows between 1997 and 2001. Dr. Wilkening graduated from the University of California at Berkeley with a PhD in Mathematics, and Dr. Fringer graduated from Stanford University with a PhD in Civil and Environmental Engineering.

Dr. Wilkening received his award at the annual DOE CSGF conference held in July in Washington, D.C., where he also presented his research. Dr. Wilkening was in Australia at the time of the conference and was presented his award in October at the Courant Institute.

For More Information

Contact Barbara Helland at helland@krellinst.org for more information regarding this award or the DOE CSGF program.

Margaret Wright of the Courant Institute (center) presents Oliver Fringer with his award at the 2003 DOE CSGF Fellows Conference. Also pictured are Barbara Helland (left) and James Corones (right) of the Krell Institute.
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<tr>
<th>Name</th>
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<td>Physics</td>
<td>1998-2002</td>
<td>Current Status: Faculty, California State Polytechnic University</td>
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<td>Eric Held</td>
<td>University of Wisconsin – Madison</td>
<td>Engineering Physics</td>
<td>1995-1999</td>
<td>Current Status: Faculty, Utah State University</td>
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<td>William Humphrey</td>
<td>University of Illinois</td>
<td>Physics</td>
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<td>E. McKey Hyde</td>
<td>California Institute of Technology</td>
<td>Applied &amp; Computational Mathematics</td>
<td>1999-2002</td>
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<td>Eugene Ingerman</td>
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<td>Applied Mathematics</td>
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<td>J Nickolas Jovanovic</td>
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<td>Lane Lisen</td>
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<td>University of Washington</td>
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<td>Todd Postma</td>
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<td>Alejandro Quezada</td>
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<td>John Ritten</td>
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<td>Robin Rosenfeld</td>
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<td>Robert Sadeghick</td>
<td>University of California – Santa Barbara</td>
<td>Physics</td>
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<td>Susanne (Essgl) Seefried</td>
<td>Massachusetts Institute of Technology</td>
<td>Aeronautics/Astronautics</td>
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<td>Marc Serre</td>
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<td>Environmental Sciences &amp; Engineering</td>
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<td>Elsie Simpson Pierce</td>
<td>University of Illinois</td>
<td>Nuclear Engineering</td>
<td>1991-1993</td>
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Gavin Comant
University of New Mexico
Biology
Advisor: Andreas Wagner
Practicum: Los Alamos National Laboratory – New Mexico
Contact: gc@unm.edu
Research Synopsis: "Why are duplicate genes so common in the genomes of unicellular eukaryotes?"; "Do duplicate genes often diverge in function?" The above questions indicate how limited our understanding of the process of conserving information stored in our genes into the enzymes and structures necessary to maintain life actually is. Using sequence analysis tools and measurements of molecular divergence, our lab has studied whether duplicate genes often show asymmetric amino acid divergence, whether the circuits often seen in transcriptional regulatory networks are evolved features, and whether duplicate genes provide the neomorphs C. elegans from loss of function in its genes.

Matthew Anderson
University of Texas
Advisor: Richard Blumrich
Practicum: Los Alamos National Laboratory
Contact: anderson@lanl.gov
Research Synopsis: "I’m interested in simple models of the physical systems that arise in robotic locomotion and manipulation. I am currently working on the problem of robotic origami folding. Origami folding is a good challenge problem for robotics because it requires complicated manipulation skills that are not well understood, for example, the manipulation of flexible objects, planning for closed loops, and planning for systems with a large number of degrees of freedom. My thesis focuses on a ‘rigid body’ model of origami. If there are crossing creases in the origami design, the ‘origami mechanism’ has the structure of a (typically compound) closed chain. The space of configurations for mechanisms of this type is quite complicated, and is usually not even a manifold."
Research Synopsis:

Lawrence Livermore National Laboratory will be the basis for re-formalizing the families, will provide us with data that will reflect the cut and paste events that protein sequences. Our alignments, which are working on a version of POA designed for databases of both splice sites and SNPs in EST sequence analysis in order to build this data structure and algorithm, which represents the true biological content of a multiple sequence alignment. We have also developed PAU, an algorithm that directly aligns PO-MSAIs to each other. This data structure and algorithm, which is in an order of magnitude faster than other methods, has been successfully employed in EST sequence analysis in order to build databases of both splice sites and SNPs in human genes. We are currently working on a version of PAU designed for protein sequences. Our alignments, which will reflect the cut and paste events that protein sequences are, will result in the multiple sequence analysis of proteins families, will provide us with data that will be the basis for re-formalizing the phylogenetics of protein families.

Boyce Griffith

Notable:

invited to and attended the 2002 Nobel Laureate Conference in Linz, Austria

Research Synopsis:

My research focuses on laser-electrode interactions in low-temperature plasmas. It is not always straightforward to determine the nature of the plasma or to detect changes in it. The goal of my research is to develop new experimental techniques to study laser-electrode interactions in low-temperature plasmas.

Benjamin Keen

Research Synopsis:

I am interested in understanding the development of numerical methods and computational tools required to simulate a three-dimensional heart model that includes realistic electrophysiology, muscle mechanics, and blood flow interaction. The goal of my research is to develop the numerical methods and computational software required to provide a platform where visualization and computation can be carried out in the context of this beating heart. One approach to modeling blood-tissue interaction is the immersed boundary (IB) method. I am developing a new parallel implementation of the IB method that aims to incorporate techniques such as adaptive mesh refinement and exact Newton methods to improve the efficiency and accuracy of the computations. Additionally, I am involved in work aimed at unifying the IB methodology with other methods to model the electrical activity of the heart. Ultimately, I envision that these two approaches will be merged into a coupled electromechanical-hydrodynamics model of the heart.

Benjamin Keen

University of Michigan

Mathematics

Advisor:

Sneaker Lam

Practicum:

Lawrence Berkeley National Laboratory

Contact:

bkeen@umich.edu

Research Synopsis:

I am interested in using level sets to achieve hard moving embedded boundaries in eminently compressible flow calculations. Level sets are a technique for tracking material interfaces in flow calculations. The level set is a function on the domain, where zero level set denotes the boundary, and it exhibits a natural equation to the system of PDEs that describes the flow that advects the function with the flow. Thus, the information provided by the level set can be fed back into the simulation, e.g. by using a different equation of state in the two regions. Ultimately, we intend that these two regions will coexist. I am particularly interested in developing efficient numerical algorithms for studying multiphase flows when these phases are involved in e.g., phase transitions.

Benjamin Keen

University of Michigan

Mathematics

Advisor:

Sneaker Lam

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Lawrence Berkeley National Laboratory

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Ahna Girishk
University of California – Berkeley
Vision Science
Contact: ahna@berkeley.edu

Benjamin Kirk
University of Texas – Austin
Advisor: Sherrilyn Ifosimah
Contact: bkirk@utexas.edu

Richmond Mills
College of William and Mary
Advisor: David Weiss
Contact: richmond@wm.edu

Notable: Received the University of California, Berkeley, Graduate Merit Fellowship Award for outstanding academic achievements.

Mary Ann Laun
University of Washington
Theoretical Physics/Chemistry
Advisor: William Nishihara
Contact: mlaun@uw.edu

Notable: Awarded the 2004-2005 Executive Fellowship for Outstanding Academic Achievement by the University of Washington.

Randall McDermott
University of Utah
Chemical Engineering
Advisor: Philip Smith
Contact: randall@ch..utah.edu

Notable: Invited to attend the 2002 Noble Laureate Conference in Lindau, Germany. Named the John Zink Award for outstanding work in combustion.

Matthew McNelly
University of Michigan
Aerospace Engineering
Advisor: Ian Boyd
Practice: Argonne National Laboratory
Contact: matthew@anl.gov

Bree Aldridge
University of Illinois
Advisor: Rajkomar Acharya
Contact: balex@illinois.edu

Kristine Cochran
Carnegie Mellon University
Advisor: Michael Lakin
Contact: kcochran@cmu.edu

Notable: Received the NSF Graduate Research Fellowship.

Amooyah Singh
University of California – Berkeley
Advisor: Michael Lakin
Contact: aamoo@berkeley.edu

Eric Sorin
Stanford University
Advisor: Daniel Soler
Contact: esorin@stanford.edu

Obioma Uche
University of Maryland
Contact: oibobi@gmail.com

Joshua Waterfall
Cornell University
Advisor: James Faeder
Contact: jwaterf@cornell.edu

Michael Wu
University of California – Berkeley
Advisor: John H. Neuendorf
Contact: michaelwu@berkeley.edu

Notable: Winner of the 2006 IEEE Systems, Man, and Cybernetics Society Best Paper Award

Annette Evangelist
University of New Mexico
Computer Mathematical Biology
Advisor: Philip Wagner
Contact: annetteev@unm.edu

Sommer Gentry
Massachusetts Institute of Technology
Advisor: Andrei Calinescu
Contact: sommer@mit.edu

Notable: Awarded the 2005-2006 Excellence in Research Award by the MIT Mathematics Department.

Robert J. Kohn
New York University
Advisor: Andrea Bertozzi
Contact: robertkohn@nyu.edu

Notable: Awarded the 2005-2006 Excellence in Research Award by the New York University Mathematics Department.

Athanassios Z. Panagiotopoulos
University of California – Santa Cruz
Advisor: Paul A. Thompson
Contact: athan@berkeley.edu

Notable: Awarded the 2005-2006 Excellence in Research Award by the University of California – Santa Cruz Mathematics Department.

Alyssa C. de los Santos
University of California – Santa Cruz
Advisor: Paul A. Thompson
Contact: alyssa@caltech.edu

Notable: Awarded the 2005-2006 Excellence in Research Award by the University of California – Santa Cruz Mathematics Department.

Jerrold Marsden
University of California – Berkeley
Advisor: Paul A. Thompson
Contact: marsden@berkeley.edu

Notable: Awarded the 2005-2006 Excellence in Research Award by the University of California – Berkeley Mathematics Department.
<table>
<thead>
<tr>
<th>Name</th>
<th>University</th>
<th>Department/Field</th>
<th>Advisor</th>
<th>Contact</th>
</tr>
</thead>
<tbody>
<tr>
<td>Paul Bauman</td>
<td>University of Texas</td>
<td>Computational and Applied Mathematics</td>
<td>J. Tinsley Oden</td>
<td><a href="mailto:pbauman@ices.utexas.edu">pbauman@ices.utexas.edu</a></td>
</tr>
<tr>
<td>William Conley</td>
<td>Purdue University</td>
<td>Nanoscale Mechanics</td>
<td>Arvind Raman</td>
<td><a href="mailto:wconley@ecn.purdue.edu">wconley@ecn.purdue.edu</a></td>
</tr>
<tr>
<td>Aron Cummings</td>
<td>Washington State University</td>
<td>Electrical Engineering</td>
<td>Mohamed Osman</td>
<td><a href="mailto:aron@turbonet.com">aron@turbonet.com</a></td>
</tr>
<tr>
<td>Krzysztof Fidkowski</td>
<td>Massachusetts Institute of Technology</td>
<td>Computational Fluid Dynamics</td>
<td>David Darmofal</td>
<td><a href="mailto:kfid@mit.edu">kfid@mit.edu</a></td>
</tr>
<tr>
<td>Sarah Moussa</td>
<td>University of California – Berkeley</td>
<td>Applied Science and Technology</td>
<td>Michael Jordan</td>
<td><a href="mailto:smoussa@uclink.berkeley.edu">smoussa@uclink.berkeley.edu</a></td>
</tr>
<tr>
<td>Tod Pascal</td>
<td>California Institute of Technology</td>
<td>Physical Chemistry</td>
<td>William Goddard III</td>
<td><a href="mailto:tpascal@wag.caltech.edu">tpascal@wag.caltech.edu</a></td>
</tr>
<tr>
<td>Emma Rainey</td>
<td>California Institute of Technology</td>
<td>Theoretical Geophysics</td>
<td>David Stevenson</td>
<td><a href="mailto:emma@gps.caltech.edu">emma@gps.caltech.edu</a></td>
</tr>
<tr>
<td>Mark Rudner</td>
<td>Massachusetts Institute of Technology</td>
<td>Physics</td>
<td>Wolfgang Ketterle</td>
<td><a href="mailto:rudner@mit.edu">rudner@mit.edu</a></td>
</tr>
<tr>
<td>Jason Sese</td>
<td>Stanford University</td>
<td>Chemical Engineering</td>
<td>Charles Musgrave</td>
<td><a href="mailto:jasese@stanford.edu">jasese@stanford.edu</a></td>
</tr>
<tr>
<td>Christina Smith</td>
<td>Vanderbilt University</td>
<td>Chemical Engineering</td>
<td>Peter Cummings</td>
<td><a href="mailto:christina.m.smith@vanderbilt.edu">christina.m.smith@vanderbilt.edu</a></td>
</tr>
<tr>
<td>Samuel Stechmann</td>
<td>New York University</td>
<td>Applied Mathematics</td>
<td>Marsha Berger</td>
<td><a href="mailto:stechman@cims.nyu.edu">stechman@cims.nyu.edu</a></td>
</tr>
<tr>
<td>Brian Taylor</td>
<td>University of Illinois – Urbana –</td>
<td>Detonation and Shock Dynamics</td>
<td>Scott Stewart</td>
<td><a href="mailto:bdtaile1@uiuc.edu">bdtaile1@uiuc.edu</a></td>
</tr>
<tr>
<td>William Triffo</td>
<td>Rice University</td>
<td>Bioengineering</td>
<td>Robert Raphael</td>
<td><a href="mailto:triffo@rice.edu">triffo@rice.edu</a></td>
</tr>
<tr>
<td>Michael Wolf</td>
<td>University of Illinois – Urbana –</td>
<td>Computer Science</td>
<td>Michael Heath</td>
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</tr>
<tr>
<td>Brandon Wood</td>
<td>Massachusetts Institute of Technology</td>
<td>Computational Materials Science</td>
<td>Nicola Marzari</td>
<td><a href="mailto:brandonw@mit.edu">brandonw@mit.edu</a></td>
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