2004 - 2005

DEIXIS

THE DOE CSGF ANNUAL

DEPARTMENT OF ENERGY COMPUTATIONAL SCIENCE GRADUATE FELLOWSHIP

Funded by:
Office of Science and
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Department of Energy Computational Science Graduate Fellowship

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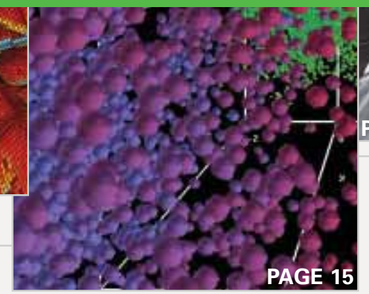
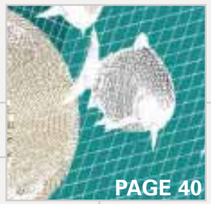


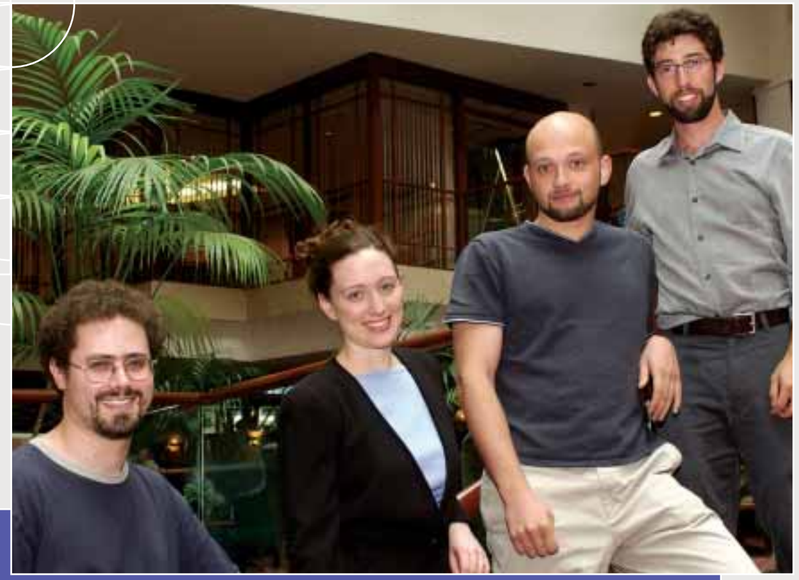


DEIXIS (ΔΕΙΞΙΣ) *transliterated from classical Greek into the Roman alphabet, (pronounced dāksis) means a display, mode or process of proof; the process of showing, proving or demonstrating.* DEIXIS *can also refer to the workings of an individual's keen intellect, or to the means by which such individuals,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

Summer of Successes

THE DEPARTMENT OF ENERGY Computational Science Graduate Fellowship (DOE CSGF) supports the education of doctoral students whose work focuses on solving complex problems in science and engineering using high-performance computing technology. These young people are already making contributions on the leading edges of science and technology. Their futures are surely bright.



Matthew Wolinsky, Sommer Gentry, Julian Mintseris, and Richard Katz take a break at the annual DOE CSGF fellows conference.

THE THREE-MONTH SUMMER practicum assignment that all DOE CSGF participants must complete is much more than a requirement. In fact, it is a tremendous opportunity to enter a Department of Energy national laboratory and pick the brains of world-class scientists who have access to extreme computing power.

Sometimes the practicum experience leads a fellow down a new path of discovery. Other times, the experience offers the right person to mentor a fellow into a new way of thinking about her research. And, almost all of the time, the experience offers the fellows a new sense of excitement about computational science and their futures as promising, young scientists.

Dances with Computers

SOMMER GENTRY

Massachusetts Institute of Technology | Sandia National Laboratories – California | Story by Victor D. Chase

Sommer Gentry was a swing dancer long before she became a fellow in the DOE Computational Science Graduate Fellowship (DOE CSGF) program, so when the demanding world of computers, mathematics and practical engineering entered her life, she did not let it replace her first love. Rather, she found a way to combine the two seemingly disparate endeavors, while approaching each with equal gusto.

By literally combining business and pleasure, Gentry, 26, was able to bring the precision of mathematical analysis to her more intuitive pastime, while working to make computers more responsive to the subtleties of human touch. In fact, the vivacious Massachusetts Institute of Technology Ph.D. candidate says, it was the requirements of the fellowship that provided her with the opportunity to combine her vocation and avocation, and that also led her to change her dissertation topic.

The Los Angeles area native earned a bachelor's degree in mathematical and computational science and a master's in operations research from Stanford University in 1998. Her affiliation with both DOE and swing dancing began right after graduation, when she took a job as a systems engineer at DOE's Lawrence Livermore National Laboratory near San Francisco, a hotbed of swing dancing, where she caught the bug.

A year later, she decided to brave the cold and moved to Cambridge, Massachusetts, to begin working toward a doctorate at MIT. At the time, her primary area of research was an esoteric field known as "inverse optimization." Then one day in 2000, on her way to class, Gentry saw a poster promoting the DOE CSGF, and her life was about to change.

"I thought, 'computational science, that sounds like me,' " said Gentry, so she applied and in 2001 was awarded a fellowship. One of her first hurdles was to satisfy the requirement that fellows include some real-world engineering classes in their curriculum. At first she tried to convince the powers that be that her prior work had satisfied that requirement, but "They said, no, no, those are math classes, you need something hands-on," she recalls. In response, she signed up for a class entitled "Space Biomedical Engineering," in which she learned about the mechanics of jointed systems, robots and humans alike. And that's where swing dancing comes in.

It's About Illusions

Swing dancing is a historical dance form, and Gentry and her husband, Dorry Segev — a surgeon and transplant fellow at Johns Hopkins Hospital, whom she met through dancing — specialize in the Lindy Hop, popular during the Big Band Era of the 1930s and '40s. In fact, Gentry and her friends attend dance events for which they dress up in clothing from that era and dance to the sounds of Benny Goodman and Glenn Miller. They also watch videos of the original swing dancers strutting their stuff, which often leads to intense discussions of who is doing what to whom in this largely improvisational dance form.

"A lot of dance is about illusions," says Gentry. "It may look like one person is pushing on another when they really aren't, or it may look like something is really light and effortless but two people are working very hard to hold each other up." Hence, she adds, "The most difficult thing to do in swing dancing is to learn how something feels."

So it was to learn from the now-departed swing dance masters of yesteryear that Gentry created her first project for the biomedical engineering class. To do so, she applied her inverse optimization expertise to calculate the forces between people by observing their moves on the videos.

This involved watching someone move and then calculating how much force was applied to make the move. "I wanted to take it out of the realm of artistic judgment and say that, physically there's something going on.

So it was to learn from the now-departed swing dance masters of yesteryear that Gentry created her first project for the biomedical engineering class.

There is a person who weighs a certain amount, and is balanced in a certain place, and either he is holding her up or he's not," says Gentry.

In doing so, she also brought peace to her swing dance community. "I just wanted to help my swing dancer friends who were arguing about what a video really showed; was this person pulling on the other person or not? I wanted to be able to give a definitive answer, and that's really what I did."

Making a science of art may also have helped Gentry and her husband place high in several international swing dance competitions. The couple came in fifth in the 2001 and 2003 national Lindy Hop championships and took first place in the 2002 U.K. Lindy Hop Open.

The judges were not the only ones who were impressed. Gentry's advisor, who saw her swing dance analysis as a rich area of investigation for a number of areas of practical applications to human/robotic interactions, suggested that she change her thesis from the theoretical to one that allows her to continue creating engineering models for swing dancing. Gentry jumped — or perhaps did a flip — at the chance.

A Mouse with Feelings

It was then that she began to dance with a PHANTOM.

In swing dancing, the leader not only guides his partner through touch but also gives signals as to what the next move will be. As Gentry puts it, "A leader is not just helping his partner by holding her up or fixing her balance, he's also telling her what move we are doing next. So there is a communications system laid on top of a physical control system, and they interact without words." This made the PHANTOM a perfect partner, since it is a haptic force-feedback device that provides virtual tactile sensation. The device includes a jointed mechanical arm that is used like a mouse but has feelings that can present forces. If a rubber ball appears on a computer screen, for example, and the user manipulates the PHANTOM to point to it, she feels as though she is pushing against a rubber ball.

Gentry carried her video analysis work several steps further by programming the PHANTOM to act as a swing dance partner through touch, even to anticipating her moves. In doing so, she helped make human/machine interactions more natural, or less machine and more human.

This work has important potential beyond dancing with computers; robotic surgery provides a case in point. In this relatively new field, robot "hands" enter the human body to perform surgical tasks under a physician's guidance. This makes surgery less invasive, since the robot requires less space in which to operate than do a doctor's hands.

Gentry envisions a surgical robot that not only follows but also anticipates the moves of the surgeon. "So if the robot can figure out that you are trying to tie a knot, it might make it easier for you to grab the free end of the suture just by pulling you toward where it knows it is. Part of that would be figuring out from the surgeon's hand motion what task he is doing, which is the same thing the follower does in swing dancing. By a little bit of push-pull, you know he's doing move A or move B," says Gentry.

Ship Shape

It was her interest in robotics that led Gentry to investigate DOE's Sandia National Laboratories, Albuquerque, New Mexico, as a place to do her required practicum. She was especially attracted to Sandia's Intelligent Systems and Robotics Center (ISRC), where a robotic ship-welding project named AUTOGEN was in progress. So last February she packed her bags and headed west.

AUTOGEN is designed to automate completely the robotic welding of ship parts. Currently, robotic welding is used for relatively simple tasks, since the time required for a human to feed instructions to a robot as to how to navigate complex nooks and crannies is frequently prohibitive. AUTOGEN would allow ship designs created on a computer to be fed directly into a computerized robot system, which would automatically calculate how best to weld the pieces together and then how best to direct the robot to do so.

For Gentry, the project was made to order, because it involved solving the same sorts of problems she dealt with in her swing dance analyses, namely, where the robot is in space at any given time.

When she arrived on the scene, AUTOGEN was already in existence, but it relied on the positioning of the robot and the piece to be welded in a fixed configuration. "I asked, 'Why don't we ask if there is a better place to put the robot and the piece in relation to each other?'" says Gentry. In response, she created an optimization routine to move the robot, or the parts, "to allow the robot to reach more of those weird corners," she explains.

Ordinarily, doing so would require inordinately large calculations. To get around this problem Gentry made some generalizations. "I abbreviated the search for ways to weld the piece by estimating how well the robot would be able to reach into hard-to-get-at crevices, instead of doing a full planning procedure. That resulted in some really neat improvements," she says.

Her Sandia practicum advisor, Arlo Ames, puts it in bolder terms. "She produced, more rapidly than I've ever seen, an answer that is a very significant piece of the overall product," he says. "AUTOGEN is a big, difficult thing. I suggested to her where to look, and she jumped in. The next thing I knew, she had code up and functional. It's working, it's very fast, very efficient, and does the right thing. The code she wrote is essentially going verbatim into AUTOGEN."

The PHANTOM Returns

Unbeknownst to Ames, a PHANTOM was delivered to a different department at Sandia while Gentry was working on AUTOGEN. She got wind of the fact and was delighted to have the opportunity to help set it up. "I jumped on the box as soon as it arrived and started running some more of my swing dance experiments," she says. Though Gentry makes it sound easy, setting up the PHANTOM requires know-how that Sandia was considering obtaining through an outside source. Instead, "just because Sommer was there, had prior experience, and is of a natural inclination to jump in and help out," the lab saved a considerable amount of money, says Ames. In fact, he says he was not even aware of Gentry's extracurricular efforts with the PHANTOM "until it was half done and people were excited," he says.

The feelings about Gentry's practicum experience are mutual. "I spent three months at ISRC. I had a wonderful time, and it gave me the opportunity to explore robotics more fully," she comments.

For his part, working with Gentry gave Ames renewed hope. "In recent years I've fallen off a lot on mentoring students because I am tired of the effort. I've gotten rather cynical about things, and the amount of my time required to get somebody up to speed was getting to the point where I was less and less willing to even try. With Sommer I have renewed enthusiasm that I can get something meaningful done with this kind of temporary workforce."

"Working with Sommer was a genuine pleasure," he adds. "I can't imagine a better working relationship; she came, she saw, she did. If I could hire her I would, but she frankly has places she's going and things she's doing."

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. Praise for the fellowship appeared in the National Science Foundation's Division of Mathematical Sciences publication *Mathematics and Science*.

PROGRAM REQUIREMENTS

Students selected for fellowships agree to undertake study and research in computational science. The program of study must provide background in a scientific or engineering discipline, computer science, and applied mathematics.

In order to be considered for the DOE CSGF, students must be U.S. citizens or permanent resident aliens and working toward a Ph.D. at a United States university.

Students applying for fellowships must be undergraduate seniors or in their first or second year of graduate study.

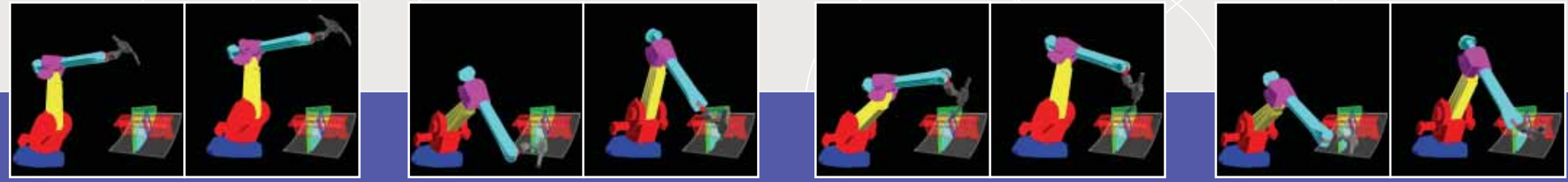
Prior to the third year of the fellowship, fellows must complete a practicum assignment at a Department of Energy laboratory. Currently, approximately 20% of fellows who graduate from the DOE CSGF program work or have worked in a Department of Energy laboratory.

DISCIPLINES PURSUED

The fellows involved in the DOE CSGF study widely varying subjects. However, they all are using high performance computing towards their research goals. Fellows' disciplines include biophysics, chemistry, biochemistry, civil engineering, computer science, aerospace engineering, applied math, physics, bioengineering, aeronautical engineering, chemical engineering, bioinformatics, vision science, computational chemistry, and computational mechanics.

These eight images are from Gentry's 2003 Sandia Labs practicum in the Intelligent Systems and Robotics Center. Gentry worked on a program called AUTOGEN, which is software to plan trajectories for robotic welding of ship parts. Each of these images includes the robot arm model in solid colors with a gray welding torch on the end, and a sample welding problem with different metal segments in different translucent colors.

The work Gentry did in her practicum added a pre-planning step to reposition the robot arm relative to the workpiece before the welding planner. In each of the pairs of pictures, default0 and better0 through default3 and better3, you can see the original placement of the robot in default and the better placement that her algorithm found. In this instance, moving the robot arm closer to the workpiece enhanced maneuverability and resulted in more weld lines being reachable by the robotic torch.



Default 0 *Better 0* *Default 1* *Better 1* *Default 2* *Better 2* *Default 3* *Better 3*

Puzzling Out the Secrets of Life

JULIAN MINTSERIS

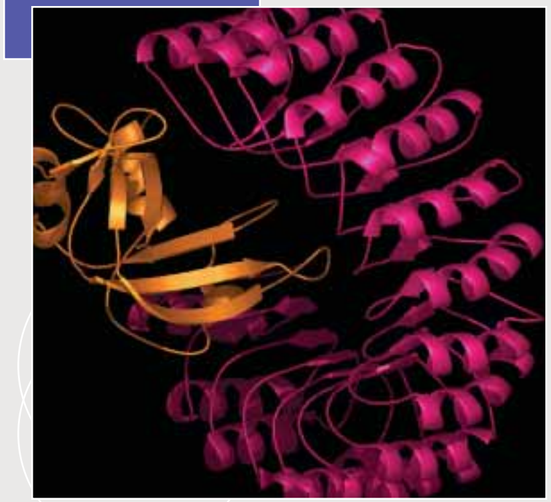
Boston University | Lawrence Berkeley National Laboratory | Story by Alan S. Brown

"Imagine approaching a large pile of mechanical parts," says DOE CSGF fellow Julian Mintseris. "You start at the bottom of the pile, put two pieces together, and if they don't fit, you throw one away and try another. If it fits, you keep both and look for another."

It sounds like a giant 3D jigsaw puzzle, but the "parts" Mintseris seeks to connect are proteins and strands of DNA. The completed puzzle will accurately represent how cells regulate themselves to adjust to changes in their environment.

The search is far from random. Instead of working with physical DNA and proteins, Mintseris uses sophisticated mathematical tools and supercomputers to reduce the guesswork of how these molecules fit together. While the task remains time-consuming, Mintseris, during his DOE CSGF practicum with Michael Eisen of Lawrence Berkeley National Laboratory, developed a technique that promises to help researchers puzzle out how proteins and DNA interact.

The enzyme ribonuclease (orange), often found in the pancreas, is involved in unwinding and cutting DNA. Here it is shown bound with an inhibitor in an unusual structure (magenta) that obstructs its function.



Twin Passions

Mintseris traces his interest in computers to his boyhood in Lithuania, when his parents returned from the United Kingdom with a PC. "The USSR made Atari-like computers, but this was much cooler," he recalls. "I started programming it when I was twelve or thirteen."

For many adolescents with a penchant for math, this might have led to a career in computers. Instead, the Mintseris family emigrated to the United States. In high school, a research paper on ethics and genetic engineering awakened an interest in biology.

He combined both interests by studying bioengineering at Cornell University and bioinformatics at Boston University. The latter is a new field that emerged because today's analytical equipment generates information about DNA and proteins faster than anyone can make sense of it. Using statistical techniques, bioinformatics sifts through these data for clues about the structure and function of genes and proteins.

In graduate school, Mintseris joined Zhiping Weng's laboratory, which uses bioinformatics to understand protein-protein interactions. In the cell, proteins act as regulators, switches that turn genes on and off. For example, a yeast cell that normally feeds on sucrose will make different enzymes if that sugar is replaced with another.

Docking Proteins

This switching mechanism is far from simple. "Some proteins interact with one or two other proteins, some with hundreds," Mintseris explains. Understanding the conditions under which they interact formed the foundation of Mintseris' practicum experience.

Proteins interact by bonding with one another through a process called docking, often depicted as matching a key with a lock. The reality is more complex.

"Imagine two cubes," explains Mintseris. "Each has six sides that can bind to any of the six sides of the other cube, so they can bind in 36 distinct ways. Now, what if they were more complex 3D polyhedrons instead of cubes? The number of distinct bonds grows very quickly."

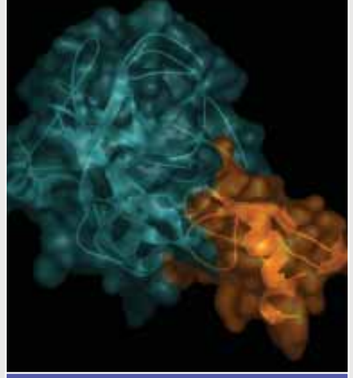
"Protein structures are far more complex than that. They're long, knotty, intertwined things made up of several hundred of 20 different types of amino acids. So imagine 200 beads on a string. But before you try to match them up, you squeeze them in your fist to make a globular cluster. Some parts repel, others attract. Somehow, though, they fit together."

To study docking, Mintseris starts with 3D structural models of proteins known to bind with one another. He then holds one protein stationary and rotates the other. "If you try to match every possible part of the surface to the other surface, the possibilities are so enormous it would take forever."

Instead, he and others in Weng's lab use bioinformatic techniques to mine databases for clues about protein docking tendencies. For example, some amino acids like to sit next to one another, and some hydrogen bonding sites have preferential attractions. He distills these insights into mathematical rules, or algorithms, that search for the most likely docking sites. The algorithms greatly reduce the number of puzzle pieces that Mintseris must sort through.

Practicum

Mintseris learned about the DOE CSGF practicum opportunity from Weng, who introduced him to Eisen at a seminar. "It was easy to tell that he was someone who thinks about a problem in the right way," Eisen recalls.



Crystal structure of the enzyme matriptase (cyan), implicated in tumor growth, bound with an inhibitor (orange) to form a complex that blocks the enzyme's activity.

"Biology is not orderly," Eisen continues. "It is the way it is because of evolutionary history. Researchers need the flexibility to listen to what it's telling us. We're explorers, not diviners of fundamental truths. It's rare to find people with math skills who can really do this."

Eisen's team probes how and when proteins bond with DNA to switch it on and off. First, though, they have to identify the binding sites. Most researchers search for them by comparing DNA from different species. After mapping out regions known to code for proteins, the regions that both DNA strands have in common are considered the most likely regulatory protein binding sites.

This type of comparison is possible because genome projects have already determined the composition of DNA. Because DNA is a simple molecule — four types of paired nucleotides (called bases) forming a well-defined double helix — it is relatively easy to line up and compare two strands.

Unfortunately, this approach does not define which protiens dock at the binding sites, though it can help to guide experiments. Mintseris thought that if he applied the protein-protein docking algorithms developed in Weng's lab to the problem, he could match specific proteins with specific binding sites.

The sheer magnitude of the problem is daunting. A 10-base-long strand of DNA carries about 1 million possible binding sites. A protein docks only at a handful of these. Past attempts to use protein-DNA docking algorithms have winnowed this down to about 1000 possibilities, but it would take years of testing to identify the actual docking sites.

Working with Eisen's team and its dedicated 40-cluster supercomputer, Mintseris began applying protein docking algorithms to DNA. He showed some success working with known proteins, but it takes months or even years to isolate a protein structure, and few are known.

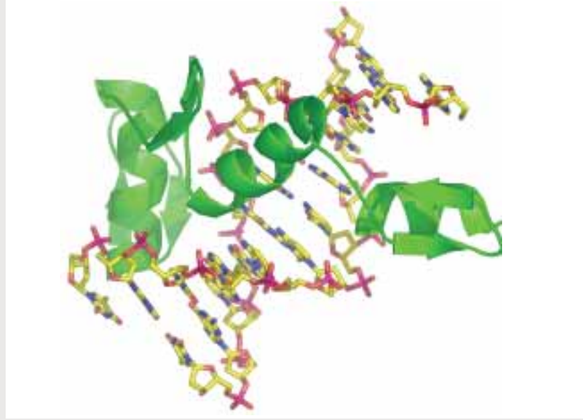
Instead, Mintseris developed a way to *guess* the structure of unknown proteins. He does this by using an algorithm to compare the composition of a target protein with that of proteins of known composition and structure. The algorithm then makes educated guesses about the target protein's structure. How well does this work? Several years ago, a research group developed a powerful algorithm that looked at experimental data and predicted the likelihood of a well-known protein family binding with hundreds of DNA sequences.

"We tested the same proteins using our algorithm and our predictions were almost as good. But we didn't use any experimental data, which took who knows how many hours to collect. We were able to predict four of the top 10 sequences known to bind that protein in real life."

The ability to automatically deduce binding affinities could help guide research for years to come. It may help scientists learn to produce proteins to control debilitating genetic diseases or turn off proteins that mediate unregulated growth such as cancer cell growth.

Mintseris is cautious. He notes that he has worked with only one protein whose behavior is relatively easy to predict. Eisen agrees, noting that it has not yet been verified experimentally, but adds that the work was "surprisingly effective" for such short development time.

Back at Boston University, Mintseris continues to sort through pieces of nature's most complex puzzle.



A protein transcription factor (green), which regulates gene expression, binding to a stretch of double-stranded DNA. The parts of proteins that bind DNA in this particular way are known as "zinc fingers" because of the way they wrap around it.

SCOPE OF PROGRAM

Since its inception, the DOE CSGF program has supported over 200 students in more than 50 universities all over the U.S. Currently it supports 71 students in 19 states: Arizona, California, Georgia, Illinois, Indiana, Massachusetts, Michigan, Minnesota, New Jersey, New Mexico, New York, North Carolina, Pennsylvania, Rhode Island, Tennessee, Texas, Utah, Washington, and Wisconsin.

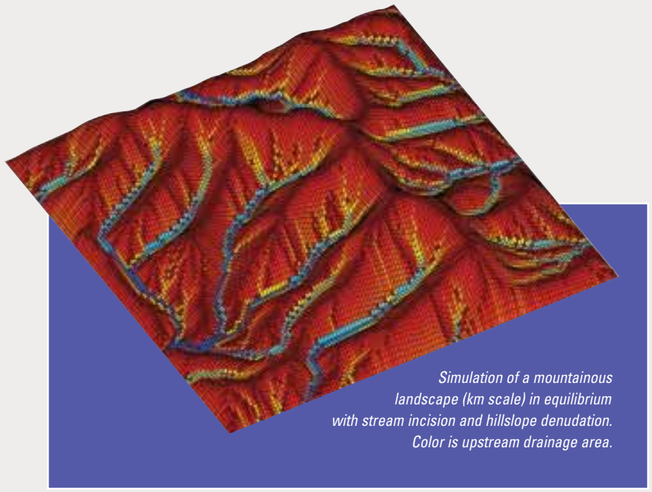
While the task remains time-consuming, Mintseris, during his DOE CSGF practicum with Michael Eisen of Lawrence Berkeley National Laboratory, developed a technique that promises to help researchers puzzle out how proteins and DNA interact.

Looking Back 500 Years to Predict Tomorrow's Weather

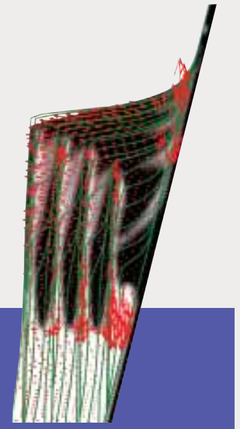
MATTHEW WOLINSKY

Duke University | Oak Ridge National Laboratory | Story by Victor D. Chase

If you want to know what the average weather was like in Old New York, say about 500 years ago, there's a good chance that David Erickson of DOE's Oak Ridge National Laboratory (ORNL) in Oak Ridge, Tennessee, could tell you. And if you want to know the probability of a drought in the region at that time, and how long it took the land to return to normal once the rains returned, Matthew Wolinsky could likely tell you that.



Simulation of a mountainous landscape (km scale) in equilibrium with stream incision and hillslope denudation. Color is upstream drainage area.



Simulation of coupled dynamic stratigraphic evolution and fluid flow. Visualization of deposit composition (grayscale sand/mud fraction), stratigraphy (green age contours), and fluid flow (red vectors).

As director of ORNL's Climate and Carbon Research Institute, Erickson is responsible for ORNL's contribution to a major national effort to create a three-dimensional computer model of the Earth's climate. Wolinsky did his fellowship practicum working on the climate modeling project under Erickson's guidance.

The 3D climate modeling project divides the planet into 150-square-kilometer grids and looks at changes in the atmosphere, clouds, continents, oceans, and rivers within each of those grids, every 15 minutes for hundreds of years. As these changes take place, there is an exchange of energy between the various elements, which controls how the atmosphere and oceans circulate and eventually determines the Earth's climate.

Using 3D modeling to examine climate changes that took place centuries ago has direct applicability to understanding existing weather patterns, such as the current global warming trend, said by many to be due to increased carbon dioxide in the atmosphere caused by the burning of fossil fuels. Numerous international bodies use the results of this work to determine policy. Erickson is, for example, a member the United Nations Environment Program on the effects of ozone depletion, and input from the ORNL project aided in the formulation of theories on global warming.

Ground Water Stream Pollution

Wolinsky, who is from Pittsburgh, Pennsylvania, and did his undergraduate work in applied mathematics and environmental studies at the University of Pittsburgh, is now working toward a doctorate in Earth and Ocean Sciences at Duke, Durham, North Carolina.

His interest in the environment is due in part to the fact that the runoff from abandoned springs draining from abandoned coal mines has led to ground water pollution of many streams in his native western Pennsylvania. As a result, his undergraduate thesis examined acid mine drainage and its effects on ground water. That tweaked his interest in geology, so when he began his graduate school career at Duke he decided to focus on geomorphology earth surface dynamics, a newly emerging field that studies the evolution of the Earth's surface and involves the study of Earth's surface and involves processes and dynamics.

"I look at what happens to the surface of the Earth, like mountains forming over different time scales, from thousands to millions of years," says Wolinsky. This includes studying how sediment from mountains is transported to oceans and becomes sedimentary basin fill, which, he says, "becomes sedimentary rocks where we now look for energy resources through offshore exploration."

To understand the structure of the landscape, Wolinsky must study past climates, the motions of the Earth's tectonic plates and the transport of the sediments that make up the Earth's surface, all of which involves modeling and data analysis, which meshes perfectly with Erickson's project.

Encouraged to Apply

Shortly after arriving at Duke in 1999, Wolinsky read about the DOE CSGF in *Physics Today* and decided to apply for a fellowship, which he was awarded in 2001. Wolinsky's new wife, Ruth, has been working toward her master's degree in environmental engineering at the nearby University of North Carolina in Chapel Hill. And although, with a new wife and a rigorous academic schedule, Wolinsky says he doesn't have much time for outside activities, he has acquired a taste for barbeque during his years down South, although the drawl is yet to come. He expects to receive his Ph.D. in 2005.

Wolinsky learned of Erickson's work while attending a seminar given by the DOE researcher, who is also an adjunct professor at Duke. Excited by the similarity of what Erickson's group is doing at ORNL and his own computational earth science and environmental work, Wolinsky introduced himself to Erickson, who subsequently encouraged him to apply to do his practicum at Oak Ridge.

Although Wolinsky's academic work involves examining changes in terrestrial mountain belts and marine sedimentary basins over thousands to millions of years, when he arrived at Oak Ridge he was put to work studying soil water retention over mere decades. Specifically, he was asked to analyze information produced by a portion of the 3D model simulations that examine how a region that has sustained drought returns to normal.

In conducting his practicum research, Wolinsky used a global model, which, says Erickson, "I encouraged him to do, because I've been pushing for students to have a global perspective and to think about how you compute the physics, chemistry and biology of our entire planet every 15 minutes for centuries. I wanted to have him realize that that is the type of research that is out there."

And although Wolinsky was not involved in creating the drought recovery model he was studying, "after seeing some of the output and looking at how the model was constructed, he contributed to possible modifications of the model," says Erickson.

Overall, he found that the practicum experience allowed him to form a revised view of DOE.

A Joint Initiative

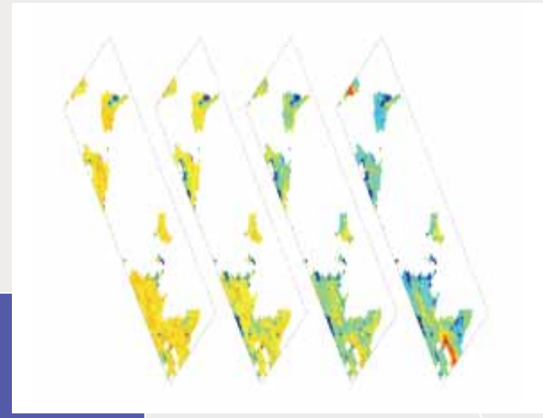
The overall 3D climate modeling initiative, known as the Community Climate System Model (CCSM), involves several DOE labs in addition to ORNL, including Lawrence Livermore, Los Alamos, Argonne, and Pacific Northwest, as well as the National Science Foundation (NSF), the National Oceanographic and Atmospheric Administration, and the NSF-sponsored National Center for Atmospheric Research, in addition to numerous universities. Yet, about one-third of the overall global century-scale calculations are being done at ORNL.

The ORNL segment of the project is being accomplished on one of the three most powerful non-classified computers in the U.S., according to Erickson, which runs at a speed of some six teraflops (six trillion calculations per second). Yet Erickson says that is still not powerful enough to examine the climate at the 20-kilometer grid resolution that he would like to see, rather than the current 150. And, he adds, "There are a lot of things that are not yet included in the models, like a fully active carbon cycle, that needs to be done." So that such factors can be included, and so that the study can be conducted on a finer scale, the DOE recently announced a $25 million grant to ORNL to begin building a 50-teraflop machine at ORNL's Center for Computational Sciences.

As part of his practicum, Wolinsky was sent by Erickson to a major conference of hundreds of CCSM participants, where he was one of the presenters of an abstract entitled "CCSM2 Sensitivity to a Single Global Soil Moisture Perturbation." The meeting, an annual affair, happened to be held in Breckenridge, Colorado, during Wolinsky's 2003 practicum.

Wolinsky, who enjoyed the interdisciplinary aspect of his practicum work, found the opportunity to attend the Breckenridge conference a particular highlight. "I got to meet a lot of people there and find out as much as I wanted about global climate modeling," he says.

Overall, he found that the practicum experience allowed him to form a revised view of DOE. "I thought there were certain problems within DOE's mission and the scientists worked specifically on those problems, but I didn't have an idea of the freedom that can be found within that," says Wolinsky. "I like the fact that Dave Erickson could get different groups together to work on a very general problem of carbon and climate that he is interested in, and that he could still be fulfilling DOE's mission."



Residual soil moisture anomaly, distributed through global terrestrial soil layers. Residual soil moisture is difference between perturbed and control Community Climate System Model (CCSM) simulations, averaged over 9 years. Research performed at ORNL.

DOE CSGF HIGHLIGHTS

- *Payment of tuition and required fees*
- *Yearly stipend of $28,000*
- *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 fellows conference with opportunities to meet other fellows and industry and government professionals*
- *Renewable up to four years*

For more information: www.krellinst.org/csgf

In the Zone

RICHARD KATZ

Columbia University | Argonne National Laboratory | Story by Katie Greene

When Computational Science Graduate Fellow Richard Katz arrived at Argonne National Laboratory last summer for his practicum, he knew that the time-honored approaches to computation in geophysics would take him only so far. Katz knew the ropes: scour the literature for colleagues working on a similar problem, adapt their computational strategy to the new problem, and then write up the code from scratch. The approach is tedious and prone to pitfalls. And Katz had taken on a problem so complex and computationally demanding that no one had yet attempted to assemble all the pieces in one computer simulation.

"I knew the physics and the geophysics," Katz says, "But I had no idea how to get enough computational power to model them. Because of that need, I think that I was in the right place at the right time with the DOE CSGF."

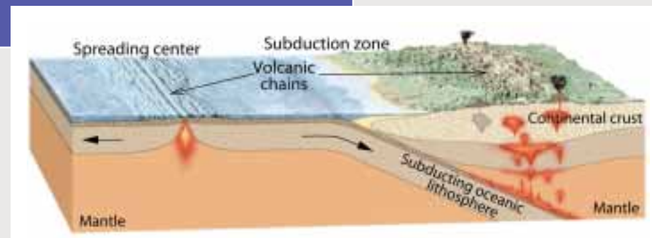
Katz studies the Earth's subduction zones — those places on the planet where the cold, hard slab of the ocean floor dives beneath the Earth's continental plates. As the slabs heat, fluids trapped in the ocean crust are released and mix with mantle rock, which triggers melting. The molten rock, or magma, then percolates upward toward the surface, where it is stored until it erupts as lava or hot ash. "But when you see the surface chemistry, all you see is a rock," Katz says. "You don't see the process that formed it." Most of the action is buried at depths of hundreds of kilometers, far below the reach of even the deepest mine. And it's difficult to reproduce the exotically hot and intense pressures of the Earth's interior in the laboratory. So Katz wants to build a computer simulation that reveals the inner workings of subduction and explains the origin of the chemical clues that rise up up from below.

But to simulate the complex chemistry and physics involved, Katz has had to set aside the "roll your own" approach to writing geophysics code and adopt the techniques and tools of advanced computational science. Katz's three-month sojourn to Argonne for his practicum made the synthesis possible, explains computational geophysicist Marc Spiegelman, Katz' advisor at Columbia University in New York. Spiegelman suggested Katz select the DOE CSGF over the NSF Fellowship because the former provided the opportunity to work with computational scientists in the national labs during the fellowship-sponsored three-month summer practicum. "There were things in computation I was interested in doing, but I didn't really have the expertise to teach him," Spiegelman explains. "So I told Richard this is the way to go — the DOE CSGF gives you the chance to go embed yourself in the expertise at the labs."

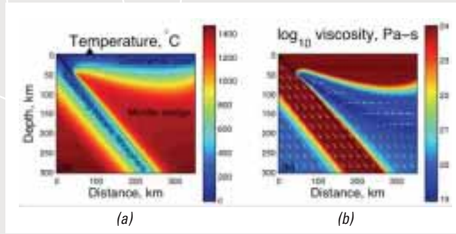
Katz selected Argonne National Laboratory in Illinois because the lab hosts a team of researchers working on the Portable Extensible Toolkit for Science, or PETSc. PETSc is a suite of general-purpose software tools which are specifically designed to solve partial differential equations — the math that describes how some natural systems change through time and space. The toolkit efficiently chops the study area up into parts and then provides the most well-known and well-studied numerical techniques needed to solve the equations specified by the researcher. It also simplifies the process of enabling the code to be solved on tens, hundreds, or thousands of computer processors at the same time. In essence, PETSc provides the equation-solving portions of a numerical simulation ready-made, allowing the user to focus on the scientific part of modeling rather than on nuts-and-bolts numerical techniques.

Within the framework of PETSc, Katz's software migrated easily into parallel. Now, he is able to increase the size of the simulated area or the complexity of the simulation as needed. He's already run problems bigger than any that fit on his Columbia desktop, but even so, they took up only a tiny portion of the available resources at Argonne. "There's just tons of room for growth," Katz says.

Armed with PETSc, Katz was poised to take advantage of another resource the lab offered: the perspective of scientists with tremendous expertise in computational science. "They saw my problem from a completely different perspective than how I looked at it," Katz says. The ability of the Argonne researchers to look at Katz's problem as an abstract mathematical idea, rather than the physical situation of rock flowing around a subducting wedge, provided an insight about how to structure the coordinate system that Katz feels he may never have made on his own. Katz later settled on another approach, but needed that first insight to get the ball rolling.



A cartoon view of Plate Tectonics (not to scale). The surface of the Earth is composed of rigid lithospheric plates. Oceanic lithosphere is created at sea-floor spreading centers where plate divergence occurs. This lithosphere moves like a conveyor belt along the ocean floor. At subduction zones, where it collides with another plate, oceanic lithosphere sinks back into the mantle. The western margin of South America is an example of a subduction zone. Typical plate motion rates are around 10 cm/year. While lithospheric plate deformation is elastic or brittle, the mantle flows viscously on geologic time-scales of millions of years. In this cartoon, orange denotes regions of partially molten mantle.



(a) *(b)*

Results from a steady-state subduction model. Light black lines mark the boundaries between the viscously deforming mantle wedge and the rigid continental and oceanic lithosphere. Flow in the mantle wedge is driven by the motion of the lithosphere. The black triangle indicates the typical position of a volcano on the surface of the Earth above a subduction zone but is not an explicit prediction of the model. (a)Temperature field in degrees centigrade. (b) Base-10 logarithm of the viscosity field is shown in color, arrows indicate the direction and magnitude of flow.

Katz proceeded to immerse himself in learning PETSc and other computational skills. By the end of the summer he had nearly completed a significant component of his project, to incorporate empirical formulas of mantle viscosity — which suggest that viscosity depends on the ambient temperature, pressure, and stress on the rock — into a simulation of mantle flowing through a subduction zone. But he had hit another sticking point. When all the contributions to the rock's viscosity were combined into one model equation, the model could not settle on a solution.

Spiegelman flew out late in the summer to meet with Katz and the Argonne researchers, another practice encouraged by the DOE Fellowship. "Together with Marc, we quickly realized a better way to combine components," Katz says. The revision worked beautifully, giving them results that matched very well with observational evidence. "So after making lots of progress looking at the problem from a computational science point of view all summer, I was able to switch back and see it again from a geodynamical point of view and make even more progress," Katz says.

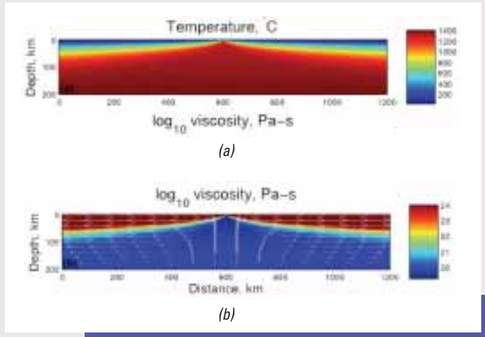
As in all good collaborations, Katz's practicum also inspired computer scientist Matt Knepley, one of Katz's advisors at Argonne, and others who worked with them to take a look at the numerical problems faced by geophysicists. "Once I got a taste of it, and did the summer work with Richard, I really felt this is something we have to get into," Knepley says.

"And that's when I started going to geosciences meetings, and we started inviting Marc [Spiegelman] to the computational meetings. I love working with those guys," Knepley says of Katz and Spiegelman. "They're deep thinkers, and they're also willing to roll up their sleeves and write a little bit of software."

Shortly after returning to Columbia, Katz put his new skills into play on a project that had little to do with his thesis work on subduction zones. During a conversation about a recently reported characteristic of mid-ocean ridges, Spiegelman suggested a simple explanation for the observations. Katz thought he could model that idea in a few weeks, and indeed by December they had written and submitted a paper that used a computational model to demystify the observations. "The speed with which I was able to do this modeling is directly related to the fact that I had all the tools that I needed and I could see exactly how to use them," Katz says.

The complete model of subduction zones is still a way off. "There's a lot of really interesting and challenging work to be done before it would even be feasible," Katz says. But he says the process has been immensely rich and rewarding. Katz knew before going to Argonne that the collaboration and the PETSc approach — divorcing the computational infrastructure from the science applications — would be helpful. "But when I actually got there and I saw the power that that gave me to do science, I realized there's no going back. This is how I need to work."

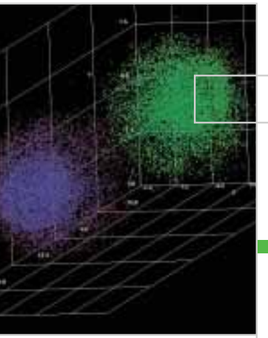
Armed with PETSc, Katz was poised to take advantage of another resource the lab offered: the perspective of scientists with tremendous expertise in computational science.



Results from a steady-state spreading center model. Flow within the domain is driven by a velocity boundary condition imposed at the surface. (a) Temperature field in degrees centigrade. (b) Base-10 logarithm of the viscosity field is shown in color, arrows indicate the direction and magnitude of flow.

By Jacob Berkowitz

Model Colliders



>> Accelerator Design
>> Verification & Validation
>> Astrophysics
>> Laser Science
>> Applied Mathematics
>> Infrastructure Analysis
>> Environmental Science
>> Transportation Engineering

UNCERTAINTY. It's a key word surrounding the next generation linear collider, or LC, currently being planned by the international high-energy physics community. Questions of design and location are almost as elusive as the Higgs boson.

But two things about this high-energy accelerator are clear: it will be very big and very expensive.

The proposed US LC design, involving two opposing linac, will stretch 14 kilometers underground — more than four times longer than the largest existing U.S. linac, the Stanford Linear Collider. Within the new linac accelerator's massive copper tubes, electrons and positrons will be accelerated to nearly the speed of light, and then smashed together, creating exotic new particles from pure energy. The results of this "tiny bang" could shed light on everything from the origins of the Universe and mass to the nature of space and time.

These results, however, will come with a massive price tag. The current estimate is $6 billion. At this size and expense, any design errors will be enormously costly, or even fatal, for this "big science" project.

Which is why, before the first shovel hits the ground, this accelerator will have an unprecedented virtual life — in large part thanks to the modeling techniques being developed by the cutting-edge Advanced Computing for 21st Century Accelerator Science and Technology project (AST).

AST is creating a comprehensive terascale simulation environment on powerful parallel computers to solve the nation's, and the world's, most challenging problems in accelerator science and technology.

"Our impact on the Next Linear Collider is significant. We are computationally modeling almost every piece of the linear accelerator," says Kwok Ko, AST's co-PI and Advanced Computations Department Head at the Stanford Linear Accelerator Center (SLAC). The Next Linear Collider (NLC) is the U.S. entry in the international next-generation linear collider race.

Started in 2001, AST's work is already proving crucial to maximizing the performance of existing accelerators, and the potential of planned and under-construction facilities and CERN's Large Hadron Collider. However, AST isn't stopping at the boundaries of the known. The group is exploring the creation of fundamentally new types of accelerators, involving lasers and plasmas, with the tantalizing possibility of desk-top models.

Accelerator Science

Particle accelerators come in two basic designs: circular and linear. There are also two distinct categories of charged particles they accelerate: electrons or hadrons. Circular, or ring, accelerators, in which energy is increased over numerous laps, are generally designed for the larger, heavier hadrons, such as protons and neutrons. Linacs are used for the lighter electrons and positrons.

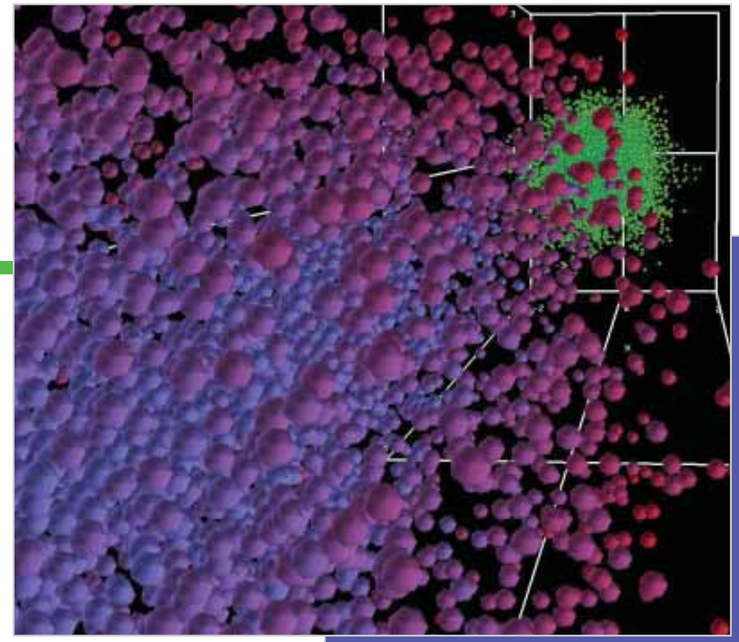
"Camera designers use computer aided tools to design systems of glass lenses that bend light in a particular way. What an accelerator physicist does is use electromagnetic cavities and magnetic lenses to accelerate, focus, and bend particle beams. And what we are doing is developing a new generation of computer codes to perform this complicated computational design," says Robert D. Ryne, AST co-PI and leader of the Accelerator Modeling and Advanced Computing Program at Lawrence Berkeley National Laboratory.

The computational models AST is developing apply to both categories of particles and accelerators. In each case, the fundamental physics and mathematical equations are applied to an accelerator's particular configuration.

The AST project is supported by the Department of Energy's Scientific Discovery through Advanced Computing (SciDAC) initiative, which harnesses the power of multidisciplinary teams to create the algorithms and codes for terascale computing.

The AST team — involving more than 50 physicists, computer scientists, applied mathematicians and computational scientists from more than a dozen universities and government labs — is developing an array of algorithms and parallel codes that cover the full scope of accelerator performance. These include simulations of beam and beam-beam dynamics, the electromagnetic system, space-charge effects (the electrodynamic effect of the particles themselves), and the overall integration of these codes.

The codes are run primarily on Seaborg, the IBM/SP Power 3 supercomputer at Lawrence Berkeley Laboratory's National Energy Research Scientific Computing Center (NERSC) facility. AST also uses the IBM/SP Power 4 computer at the Oak Ridge National Laboratory's Center for Computational Science.



Visualization of two bunches approaching one another in a high energy collider. The self-consistent simulation of beams in colliders over millions of revolutions demands use of the most advanced high-end computing resources.

Ko says this massive computing power has made modeling a "core technology" in accelerator design.

"It's not only that we have the computers to simulate the design, but we can do it so much faster and more accurately than in the past," says Ko. He notes that the Next Linear Collider models he developed in the mid-1990s that ran 24/7 for months on workstations now take an hour to run on a NERSC supercomputer, and have 10 times greater accuracy.

"Accelerators and accelerator modeling are crucial to the future of DOE and U.S. science. In DOE's Facilities for the Future of Science 20-Year Outlook, nearly half of the priorities are accelerator facilities," says Ryne.

Keeping Particles In Line

The SciDAC AST project has already made major advances in modeling beam-beam interactions, wakefield effects, and the integration of simulation components.

AST is creating a comprehensive terascale simulation environment on powerful parallel computers to solve the nation's, and the world's, most challenging problems in accelerator science and technology.

COLLABORATORS

Robert Ryne is a group leader in the Accelerator Modeling and Advanced Computing Group at Lawrence Berkeley National Laboratory (LBNL) and is also a co-Principal Investigator of the Department of Energy SciDAC project, "Advanced Computing for 21st Century Accelerator Science and Technology."

Dr. Ryne's research interests include beam physics, parallel computing, and techniques for the numerical simulation of classical and quantum dynamical systems. He is an active member of the U.S. accelerator physics community.

Dr. Ryne received his B.S. degree in physics from the University of California at Berkeley in 1981. He received his M.S. and Ph.D. degrees in physics from the University of Maryland at College Park in 1987, specializing in accelerator physics. His thesis research, under the direction of Professor Alex Dragt, was on the Lie algebraic treatment of space charge. During this period Dr. Ryne also contributed to the development of the MaryLie beam dynamics code.

Kwok Ko joined the Applied Physics Operation at Science Applications International Corporation (SAIC) in 1981 as staff scientist and engaged in research ranging from ELF generation in space plasmas to high-power devices such as gyrotrons and gyroklystrons. Since 1989, he has been at the Stanford Linear Accelerator Center (SLAC), where he now heads the Advanced Computations Department (ACD), a new department he formed in 2001 to focus on high performance computing. He was a co-PI on the DOE Accelerator Modeling Grand Challenge (1997-2000) and currently co-leads a large multi-institutional project funded by the DOE Scientific Discovery through Advanced Computing (SciDAC) program to develop advanced accelerator simulation tools for use on terascale computers.

Dr. Ko received his Ph.D. in Plasma Physics from the University of Southern California in 1979. His graduate studies centered around theoretical and numerical analysis of nonlinear plasma wave phenomena. He was a postdoctoral fellow at the MIT's Research Laboratory of Electronics, where he worked on radiofrequency heating of fusion plasmas.

Further Reading:

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PRACTICUM COORDINATOR

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A prototype of the NLC accelerating structure consisting of 55 cavities.

Below: Two of the 55 cavities. Beam travels through the center aperture.

One of the project's major successes is the development of the BeamBeam3D code to model and understand the interactions of colliding beams. Developed by the Berkeley Lab's Ji Qiang, the code has been used to model the performance of Fermilab's Tevatron, the world's highest energy hadron accelerator currently used for experiments, as well as collisions in SLAC's Positron-Electron Project (PEP-II) and Brookhaven National Laboratory's Relativistic Heavy Ion Collider.

The BeamBeam3D code was recently successfully used to perform the first one million turn, one million macro-particle fully self-consistent simulation to study beam-beam interactions in CERN's Large Hadron Collider, scheduled to go on-line in 2007.

As accelerators grow in size and energy level, one of the major challenges is managing the electromagnetic effects of the particles themselves. High-energy accelerators can have dozens of bunches of particles in a line, like boats in line on a river. The electromagnetic wake, or wakefield effect, from the first bunches can skew the path of the following particles.

"Think about it," says Ko. "In the Next Linear Collider a charged particle has to go in a straight line for six kilometers in order to collide with the opposing charge. How do you keep it in line over that enormous distance?"

Ko is leading a group that's developing electromagnetic codes to model wakefield effects. Recently, his group performed the first complete wakefield analysis of the proposed NLC linac structure, using a 3D electromagnetic code they've developed called Omega3P. The model involved solving the largest equation the group has ever tackled. The simulation required 700 gigabytes (GB) of memory and took 56 hours on 1024 processors on the IBM/SP3.

Along with modeling wakefield effects, the Omega3P code may also reduce the margin of error in frequency deviations in DOE's planned Rare Isotope Accelerator (RIA), thereby reducing the accelerator's price tag. The RIA design currently calls for numerous tuners to counter-balance frequency variations, of about one percent, in the accelerator cavities. However, with Omega3P the AST team believes they can achieve a ten-fold improvement in frequency accuracy, thereby significantly reducing the number of tuners required and thus the project's overall cost.

Ryne and Ko emphasize that in order to succeed, this level of terascale computational science relies on close collaboration with computer scientists to optimize the use of computer architecture and handle the enormous data management and transfer issues. As a SciDAC project, Ryne says that AST receives "red carpet treatment" from the NERSC User Services group, including AST's assigned staff member, Richard Gerber.

"Richard Gerber has helped us in many ways, but particularly with regard to performance analysis and enhancement. In one case he boosted the performance of a code to 25 percent of the theoretical peak."

The AST project also benefits from being able to divide problems into dozens of component parts, each tackled by a nationwide team of experts.

"We take a modular approach," says Ryne. "Individual components are developed by team members at Brookhaven, Fermilab, Los Alamos, the University of Maryland, UCLA, the Berkeley Lab, and elsewhere, and are brought together in a unified, coherent framework."

One successful application of this approach, a framework called Synergia, was developed by a team headed by Fermilab's Panagiotis Spentzouris and is now being used to improve the performance of the Fermilab booster. AST is also being supported by experts in areas such as parallel eigensolvers and sparse linear solvers, partial differential equation solvers, meshing technologies, statistical methods, and scientific visualization.

Exotic Accelerators

Along with modeling existing and planned accelerators, AST members are also exploring "exotic concepts" for new breeds of high-energy accelerators that could transform the scientific and technical use of accelerators.

The project's Advanced Accelerator Modeling component is led by UCLA's Warren Mori, who heads a team that also involves members from University of Southern California, the Berkeley Lab, and Tech-X, a private company. Their research includes modeling the use of plasmas and high-energy lasers to provide unparalleled rates of particle acceleration and so potentially to make smaller, cheaper and much more widely accessible accelerators.

Inspired by the advent of terawatt, table-top lasers, the goal is to create the hot-rod version of an accelerator: high-speed over a short distance. Current accelerators have an acceleration gradient ranging from a few million volts per meter (MV/m) to a few tens of MV/m. This requires large machines in order to provide the distance to achieve high-energy beams.

"If you use these extremely innovative techniques of advanced accelerator concepts, where you harness the high fields present in lasers and plasmas, you can get to gradients 100 or 1000 times beyond conventional technology," says Ryne.

This would reduce a kilometer-long accelerator to a single meter in length, opening the way to a desk-top model that could be used in hundreds of labs around the world. It's a vision of the future that for Ryne and Ko shows that computational science can not only support the design of accelerators, but indeed radically change our understanding of what accelerators can be.

Above: Computer model of the NLC accelerating structure.

FORGING THE ACCELERATOR MODELING PATH

>> ***Kwok Ko and Robert Ryne, co-Principal Investigators of the Advanced Computing for 21st Century Accelerator Science and Technology project (AST), each have 20 years of experience with accelerator modeling. In their field, that's the equivalent of having driven since the days of the Model-T.***

Now, they say, the DOE's Scientific Discovery through Advanced Computing (SciDAC)-supported AST project is catalyzing two decades of incremental growth to make accelerator modeling a truly collaborative affair.

When Ko started at the Stanford Linear Accelerator Center (SLAC) in 1989, he was one of a handful of computational scientists there. Back-of-the-envelope calculations — elegant and highly intuitive — were the reigning tool for accelerator theoreticians. He lobbied for, and won, SLAC's first IBM RS 6000 workstations.

"In those early days I pushed for using simulation to get results that could go right into design," says Ko, who now heads a department of 13 staff physicists, computer scientists and mathematicians, and three graduate students.

For Robert Ryne, DOE graduate internships played a central role in turning an academic career path in light optics into a leading role in computational beam optics at a national lab. While working on his Ph.D., Ryne spent summers as an intern in the Accelerator Technology Division of Los Alamos National Laboratory.

"My graduate research assistantships at Los Alamos taught me what an exciting place a national lab can be, and because of those early experiences I have been with the national labs ever since," says Ryne.

Both he and Ko say that the SciDAC program is revolutionizing the way high-performance accelerator modeling is done.

"A supercomputer is a very powerful tool," says Ko. "But this powerful tool requires a multidisciplinary team culture to maximize its use. SciDAC is creating that culture."

Wakefields generated by a beam traveling down the NLC accelerating structure as simulated with Tau3P, another SLAC code developed under SciDAC.

Science of Prediction

IMAGINE BEING ASKED to stake your country's security and reputation on decisions concerning the performance, reliability, or safety of nuclear weapons. Only there's one catch: In many cases you cannot directly test these weapons; and in the cases where you can test, the costs are so prohibitive that you are limited as to which tests to perform.

If you are a computational scientist, you can use computer models to simulate what might happen in various scenarios and then report your predictions. But, since the uncertainties can be quite large, how do you respond when asked, "How confident are you in your predictions?" or "How do you know your models match reality?"

The question of how to address uncertainty in complex computational physics and engineering simulations of nuclear weapon systems has come to the forefront as performing underground tests on nuclear devices is banned under the Comprehensive Nuclear Test Ban Treaty. It is the mission of the National Nuclear Security Administration's Stockpile Stewardship Program to develop and implement science-based methods to ensure any decisions about the management of the U.S. nuclear stockpile are based on the best available science and data. The program, a collaboration among Sandia National Laboratories, Albuquerque, New Mexico; Lawrence Livermore National Laboratory, Livermore, California; and Los Alamos National Laboratory, Los Alamos, New Mexico, has pioneered a rigorous system of verification and validation (V&V) that allows code developers, code users and decision makers to have confidence in the accuracy of their computer simulations necessary for this goal.

"Historically, we have approached important stockpile issues through testing," says Martin Pilch, Verification and Validation Program Manager at Sandia. "Now that there is no testing, the open question becomes: 'Can we do a better and more credible job using modeling and simulation?'"

Pilch directs the efforts of a group of 50 physicists, engineers, mathematicians and software developers at Sandia whose mission it is to ensure the credibility of simulated nuclear weapons tests.

There is a strong philosophy in the U.S. nuclear weapons program of safety, security, and reliability of the weapons, says Pilch. "One role of the Laboratories is to continue to ensure the weapons are stored and, when necessary, transported as safely as possible."

A major aspect of this stewardship is to anticipate worst case scenarios and try to ameliorate any potential consequences. To do that, the Department of Energy's Advanced Simulation and Computing program (ASC) develops simulations to study nuclear weapon design and manufacturing processes, along with weapon response in accident scenarios, as well as weapons aging issues.

For example, one area of interest is how a weapon might react if it found itself in a fire, such as during a transport accident. This is one area in which testing, although possible, is quite limited because of costs.

"The question is do we really understand how this system is going to behave in unusual situations," says Pilch.

There are two broad classes of modeling required to understand what would happen, says Pilch. One involves modeling fires, which provides heating to the weapon, and the second involves how the weapon might respond to a fire environment. Each class of modeling has its own computer simulation program.

A major aspect of this stewardship is to anticipate worst case scenarios and try to ameliorate any potential consequences.

The Fuego simulation program was specifically designed to model an abnormal fire environment in high-consequence accident scenarios that may arise during nuclear weapon transport. The abnormal environment is defined by the fire, turbulent reacting flow field that provides heat convection and thermal radiation. Likewise, the Calore program simulates the thermal response of the weapon. Calore is a software tool for performing large-scale, nonlinear thermal analysis. Both Fuego and Calore are being developed by computational scientists in the Engineering Sciences Center at Sandia. These tools are components of a larger scientific software system called SIERRA, an object-oriented, unstructured grid framework for multiphysics analysis that provides support services such as mesh adaptivity, parallel communication, linear solvers, and data transfer.

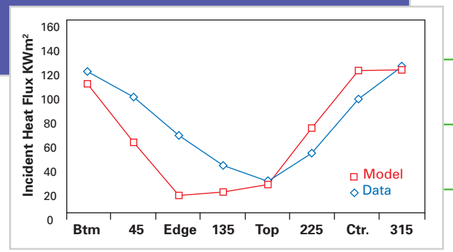
The types of analyses relevant to fire environments include nonlinear heat conduction, enclosure radiation on dynamic surfaces resulting from material removal, thermal contact resistance,

Full-scale accident.

System qualification for large fires that can result from transportation accidents.

Controlled experiments are crucial for understanding and prediction.

Code validation of heat flux to systems at real scale.



MARTIN PILCH

Martin Pilch is currently the V&V Program Manger for the Advanced Simulation and Computing (ASC) Program and a line manager of the Validation and Uncertainty Quantification Department in the Engineering Sciences Center at Sandia National Laboratories. He received his Ph.D. in nuclear engineering from the University of Virginia and is certified as a Project Management Professional (PMP) by the Project Management Institute. He spent the first nineteen years of his career developing and validating models for severe accident issues associated with the operation of nuclear power plants. During this time he participated in and led major activities using a risk-informed approach for addressing and resolving safety issues that arose as a consequence of the accident at Three Mile Island. For the last five years he has managed the V&V program at Sandia, with a goal of establishing credibility in the use of modeling and simulation for nuclear weapon issues.

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and chemical kinetics associated with decomposing materials. To make the simulations work requires coupling between mechanics of disparate length and time.

All of the computer codes, which are the products of much code development to get them to work together properly, have been designed for use on large, parallel supercomputing platforms.

"What we are doing is pushing very complex computational models to their limit," says Tim Trucano, a mathematician who specializes in computational physics and uncertainty estimation at Sandia. "We ruthlessly ask the most demanding questions we can of these computational models to be able to fully understand what's really going on and have confidence in the answers."

To be able to do this in a credible way involves a high level of physics fidelity and geometric fidelity in the models and requires very large computers *[see sidebar on Red Storm]* with the ability to do many large calculations to help quantify uncertainty. Proper use of this modeling requires quantifying the uncertainty in the predictions. To do this may require hundreds of simulations with changes to the various parameters reflecting the uncertainty in the use of the model.

"Once you acknowledge that there are high consequence issues that you want to address with modeling and simulation, then the next step is to question the credibility of the calculations that you have produced," says Pilch.

There are a number of elements to this, explains Pilch. One is verification, which answers the question: Are you solving the equations correctly? There is also validation, which is comparison with experimental data to answer the question: Are you solving the right equations? Verification is further divided into the questions of whether the solution algorithms are correct; whether the associated software is bug-free, primarily a software engineering challenge; and finally, how accurate specific calculations are.

"Because we are making such very high-end use of computer codes, the issues of verification and validation of those models is ratcheted up a level," says Pilch. "And so the level of formalism that we are bringing to that is well beyond what's ever been used before."

The size and number of the required calculations has its roots in the fundamental logic of V&V, which requires careful study of both the accuracy of the codes in specific applications and the effect of uncertainty in application calculations, explains Trucano.

"One of the major issues to address is how to believe that you are modeling correctly when you cannot obtain sufficient (sometimes any) experimental data for the particular event you are modeling. Your only recourse is to draw conclusions based on related experiments that you are able to perform," says Trucano.

For example, says Pilch, it is possible to take the nuclear material out of a warhead and conduct a full-scale (fire) test on that warhead, but perhaps only one such test might be possible because of cost. The goal is to prepare ahead of time as to get the maximum possible information from the test by going into the test with a good understanding of what might be expected to occur through the use of simulation.

"What we are doing is contributing careful, rigorous information that is going to allow more conclusions to be drawn from a single system test," says Trucano. "We are building more science into the process from the very beginning so that you have a firmer science underpinning for complex system tests, which will allow you both to reduce the number of tests and get a lot more information out of them."

While such rigor is essential in a high-consequence environment such as nuclear weapons systems, the V&V program being implemented through ASC is just as applicable to modeling other complex phenomena that require nonlinear physics, stochastic-like behavior, and the need for many spatial and temporal scales, such as climate modeling, protein folding or even economic predictions.

"One of our expectations for this V&V program is to offer a national paradigm, particularly for issues that might be facing the DOE in the future," says Trucano. For example, when scientists make climate predictions based on modeling systems, some of the same questions that the ASC V&V program addresses are likely to be asked. If national policy is to be based on computational models, it is only natural to want to be as confident as possible in those predictions and then to make an informed decision. A V&V program goes a long way to helping ensure that confidence.

"It is standard practice to be able to manage risk to the extent that if you get enough knowledge, you might still be willing to make a decision about what you don't know," says Trucano. "What we try to do more than anything else is to make sure when the day is done, you know what you have and you know what you don't have and you understand what the likely implications of that are."

RED STORM RISING

>> ***The computing requirements for the nuclear weapons stockpile is enormous when considering the need for three-dimensional geometries and full physics modeling of the governing physics and engineering. "This means that the computational requirements for accomplishing verification and validation (V&V) grow to the same degree as the calculations that must be subjected to V&V," says Tim Trucano, a mathematician who specializes in computational physics and uncertainty estimation at Sandia.***

The computing demands of V&V are large, both in terms of the size of the needed calculations, called "capability computing" in the jargon of this community, and in terms of the numbers of calculations, called "capacity computing". V&V places a large demand on ASC's current generation computer systems.

But help is on the way, as a unique collaboration between Sandia and Cray Incorporated has resulted in a faster, yet smaller and less expensive supercomputer called Red Storm. It is the latest computer that will be enlisted in performing the calculations specific to the ASC V&V program.

Design innovations permitted completion of the machine, from concept to assembly, in less than 30 months, compared to the usual four to seven years from concept to first product on a new supercomputer.

Red Storm is composed of 10,368 AMD Opteron processors and is expected to run seven times as fast as the ASCI Red computer system. It has a theoretical peak of 41.5 teraflops (trillion operations/second), and is expected to be fully operational at Sandia in January 2005, says Bill Camp, Sandia's Director of Computation, Computers, Information and Mathematics. Red Storm has unique characteristics: it is scalable from a single cabinet (96 processors) to approximately 300 cabinets (30,000 processors).

Massively parallel supercomputers, three-dimensional and full physics codes, and the supporting infrastructure continue to be the core of the ASC program. The NNSA labs have taken the lead, partnering with the US supercomputing industry, to create the computing power required for their advanced applications.

"But the truth is, as soon as Red Storm is up and running, our applications will have it running to capacity," says Trucano. "There is no end in sight to the expanding needs of computing capability within the ASC program, and V&V mirrors these needs."

storm

By Jacob Berkowitz

Modeling Star Power

THEY ARE ESSENTIALLY MASSLESS particles, so elusive that trillions of them pass right through the Earth every second as if our globe were a cosmic illusion. Yet inside a star more than ten times as massive as the Sun, these elusive particles — neutrinos — will determine the fate of that massive star. Barely perceptible on their own, nearly infinite numbers of them will fuel the biggest explosion in the Universe: a core collapse supernova.

Modeling the neutrino production, transport, and interaction is what makes these cosmic firecrackers so difficult to model numerically. Which is why Mezzacappa is leading the TeraScale Supernova Initiative (TSI). Sponsored by the DOE Office of Science's Scientific Discovery through Advanced Computing (SciDAC) Program, TSI is a broad multidisciplinary project with a straightforward long-term goal: create realistic 3D models of core collapse supernovae.

"And one of the most amazing things about core collapse supernovae and modeling them is that the fate of a massive star, so enormous that if it were placed where the Sun is it would envelope the Earth, depends on the state of the microscopic nuclei in its dying core. This means we have to model physics on all scales, from nuclear to stellar scales," says Dr. Anthony Mezzacappa, theoretical astrophysics group leader at DOE's Oak Ridge National Laboratory (ORNL).

While the goal is clear, the process and the science are enormously complex. Including its collaborators, TSI involves almost 100 astrophysicists, nuclear physicists, applied mathematicians and computer scientists and staff at nearly 30 institutions in eight countries. "We're pushing all the frontiers of science, computer science and mathematics at once," says Mezzacappa.

As a result, TSI's supernova models will provide a detailed theoretical framework that will help guide future astronomical observations — including observations of gravitational ripples in space-time.

Cosmic Labs

Core collapse supernovae are atomic factories: they are believed to be the source of about half of all the elements heavier than iron, and the major source of all elements between oxygen and iron, in the Universe. But beyond producing the building blocks of matter, what makes them particularly scientifically intriguing is the way they explode.

There are two broad categories of supernovae. Core collapse supernovae are the big sisters of the other type of stellar explosion, the Type Ia supernovae. The latter type is the thermonuclear explosion of white dwarfs — carbon-oxygen stars slightly more massive than the Sun. (They're also the focus of computational modeling similar to TSI by the University of Chicago's Flash Center, a TSI collaborator.)

Unlike the situation with Type Ia supernovae, the explosion of a core collapse supernova (from here on just "supernova") is driven mostly by neutrino heating, with turbulent, magnetic, rotational and gravitational forces also playing a role. The massive star (more than 10 times the mass of the Sun) is ripped apart as a result of a sequence of events triggered by the gravitational collapse, followed by rebound, of its iron core, which in turn generates a torrent of neutrinos. It's a dizzyingly complex explosion dynamic that depends on everything from the quantum dynamic state of the nuclei to the general relativistic flow of the exploding, turbulent, stellar core, driven by a shock wave created by the collapse.

"These supernovae can serve as a laboratory for physics that can't be replicated on Earth," says Mezzacappa. "But the caveat is that your models have to be good. If the models are sophisticated, we'll be able to extend fundamental physics from them."

TSI's supernova models are providing detailed theoretical frameworks for terascale computing and astrophysical observations – including pointing the way to the first measurements of gravitational ripples in space-time.

The pioneering numerical simulations of supernovae were done in the mid-1960s by Stirling Colgate at Los Alamos National Laboratory and Jim Wilson at Lawrence Livermore National Laboratory.

However, the evolution of these models is "directly linked to supercomputing power," says Mezzacappa. "To do really accurate 3D supernova modeling will require 100 Teraflops sustained speeds and beyond, and that requires a petascale platform."

It's these 3D models that will provide the level of detail required to fully understand a supernova's explosion mechanism.

Neutrino by Neutrino

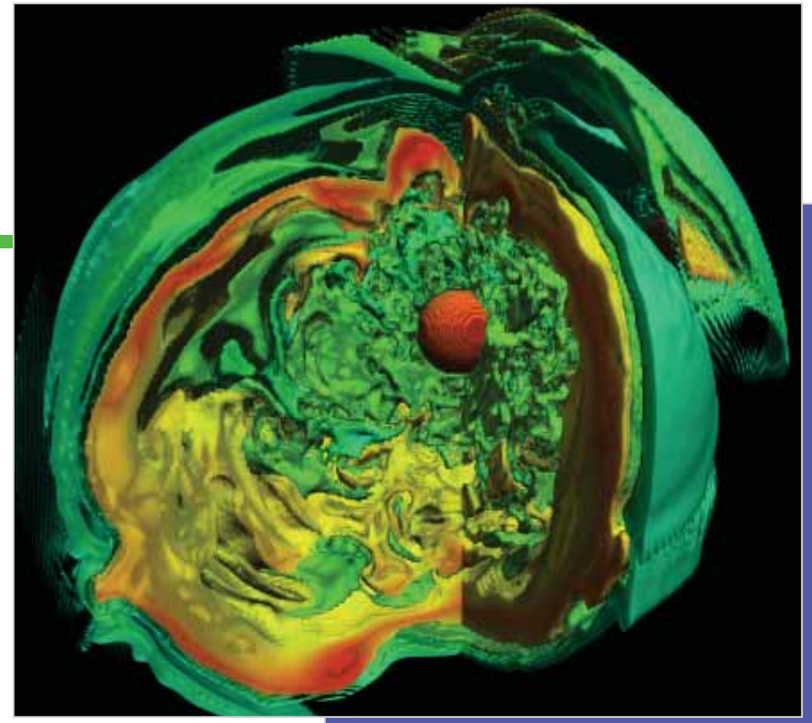
The TSI team is taking a multi-pronged approach to its ultimate goal by simultaneously finessing the various components of 1D, 2D and now early stage 3D simulations. This involves developing and integrating algorithms and codes on a step-wise journey to finding the detailed recipe for a stellar core collapse explosion.

"The neutrino transport is the most important component of the supernova model," Mezzacappa says.

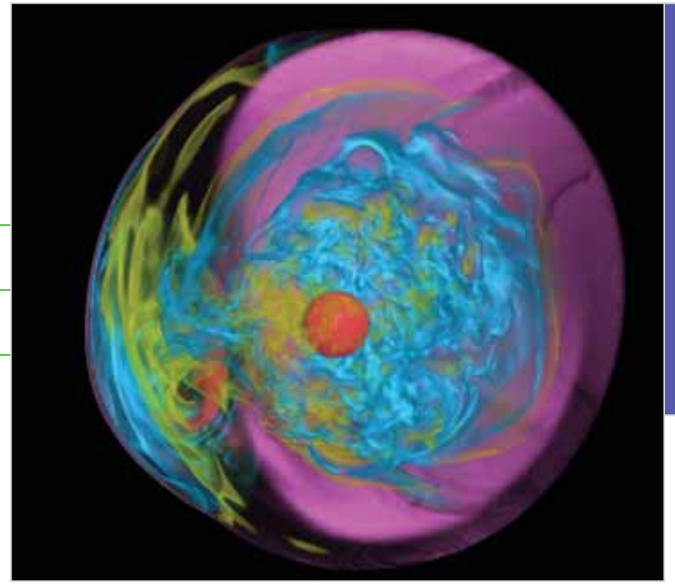
The challenge is that modeling this neutrino production and transport is a 7D problem. When the stellar core collapses, it produces a proto-neutron star that radiates 10^{57} neutrinos per second and 10^{45} watts that power the shock wave. The initial location of the shock depends on the electron capture rate of the nuclei in the iron core during collapse. This in turn depends on the quantum mechanical energy levels of these nuclei.

"Getting the right electron capture rate means knowing how to compute the correct nuclear state," Mezzacappa says.

In 2003, TSI's astrophysics team, led by ORNL's Raphael Hix and post-doctoral research associate Bronson Messer, performed the



This is a snapshot visualization by Ross Toedte (ORNL) of data from a three-dimensional simulation of the turbulent fluid flow developing in the center of an exploding star. The simulation was performed by John Blondin (NCSU) at the ORNL Center for Computational Sciences, under the auspices of the DOE SciDAC-funded TeraScale Supernova Initiative led by Tony Mezzacappa (ORNL).



This is a high-resolution rendering completed by Kwan-Liu Ma of UC Davis. It shows the development of an instability of a shock wave in a simulation of an exploding star by John Blondin of NC State as part of the TeraScale Supernova Initiative led by Tony Mezzacappa of ORNL. The shock wave is ultimately responsible for generating the explosion and is represented by the surface in the rendering. The detailed turbulence of the flow below the shock is evident. The shock wave becomes more and more distorted with time, leading to increasingly turbulent flow beneath it.

first 1D stellar core collapse simulations with state-of-the art neutrino transport and electron capture physics. The electron capture physics was developed in part by TSI's nuclear physics group, including ORNL's David Dean as well as Karlheinz Langanke of the University of Aarhus in Denmark and his European collaborators. The results showed that the more sophisticated models do indeed produce significantly different stellar behavior and led to two publications in *Physical Review Letters.*

These 1D simulations are enabling the TSI team to develop accurate electron capture rate tables that will act as premodeling input data for multidimensional models.

"The 1D models are now very sophisticated," says Mezzacappa. "But they're spherically symmetrical models. There's something missing — they don't explode."

Maximizing Terascale Models

Elucidating the role of neutrino transport and the importance of radiation hydrodynamics in supernova simulation has led the group to explore a variety of computational architectures to maximize the various codes in their evolving models.

Most of the codes are running well on IBM Power3 and Power4 platforms at the ORNL's Center for Computational Science and at Lawrence Berkeley Laboratory's National Energy Research Scientific Computing Center (NERSC) facility.

However, Mezzacappa notes that the TSI team is gradually porting several of its codes to ORNL's Cray X1.

"The Cray X1 has a very different memory/processor configuration and the memory bandwidth is very different. So it's proving, as we move one code at a time, to be a very promising platform," says Mezzacappa.

This has proved to be the case with the simulation of radiation transport in the supernovae.

"It's difficult to model 3D fluid flow, and it's very difficult to model magnetohydrodynamic flow. But radiation hydrodynamics — where radiation transport intersects with the fluid flow and helps drive it — is an absolute killer," says Mezzacappa.

The TSI team is tackling this by use of a suite of codes that includes the Virginia Hydrodynamics (VH-1) code co-developed by North Carolina State University's John Blondin, a TSI co-Investigator. The code is based on an algorithm that involves a data transpose, or switching the data on the processors of a parallel platform.

"When you have this kind of algorithm for the hydrodynamics it's much more effective to have fewer, more powerful nodes, as in the case of the Cray X1," says Mezzacappa.

However, although Blondin was able to run improved simulations of developing shock instabilities in supernovae on the Cray X1 "he was temporarily dead in the water" when it came to analyzing the results, says Mezzacappa. Each of Blondin's simulations produced a terabyte of data, too much to transfer to his North Carolina State lab for analysis on his cluster.

To solve this terascale bottleneck, Micah Beck and Scott Atchley, networking faculty and staff at the University of Tennessee, used Logistical Networking hardware and software tools to create a high-speed pipeline (ten times faster than existing ones) between ORNL and North Carolina State University.

Multidisciplinary support has also greatly improved the speed of TSI's unique code for general relativistic Boltzmann neutrino transport and neutrino radiation hydrodynamics in 1D models. Improved parallel algorithms were developed by Ed D'Azevedo, an applied mathematician at ORNL. The code itself was optimized with input from ORNL's Pat Worley and Kumar Mahinthakumar of North Carolina State, who are both members of the Performance Evaluation Research Center (PERC), a SciDAC-supported code optimization group. Finally, the code was ported to the Cray X1.

"With the port to parallel architectures and these algorithmic and performance advances the code burns now," says Mezzacappa.

Along with these improvements to the 1D model, Mezzacappa says, Doug Swesty and Eric Myra, both TSI members at the State University of New York at Stony Brook, are now running the first 2D models with multi-neutrino energy transport, and he hopes that by 2005 the TSI team will have fully realistic 2D models.

Models Meet Matter

The data from these models will help astronomers when they look to the stars.

TSI's work will provide detailed predictions of gravitational waves from supernovae that could be used by LIGO, the Laser Interferometer Gravitational Wave Observatory. LIGO's goal is to detect gravitational waves of cosmic origin, literally ripples in the structure of space-time.

The two LIGO observatories are located in Livingston, Louisiana and Hanford, Washington; each houses a laser interferometer, consisting of mirrors suspended at each of the corners of a gigantic L-shaped vacuum system, measuring 4 kilometers (2.5 miles) on each side. Precision laser beams in the interferometer will sense the mirrors' infinitesimal motions (less than one-trillionth the width of a human hair) caused by gravitational waves.

Core collapse supernovae are considered a prime source of powerful cosmic gravitational waves.

"Our hope is to provide LIGO with the theoretical templates of what the gravitational signal should look like. Hopefully, that's particularly useful to LIGO as they search for gravitational waves from supernovae," says Mezzacappa.

Gravitational waves were first predicted by Einstein's Theory of General Relativity in 1916, when the technology necessary for their detection did not yet exist. Now, almost a century later, it could well be thanks to the simulation of stellar explosions on Earth that LIGO will know when it really receives its first cosmic bump from a core collapse supernova.

A SCIENTIFIC STAR

>> ***The TeraScale Supernova Initiative (TSI) isn't just in pursuit of new knowledge; it's a new way of doing science that's receiving rave reviews and results.***

TSI is a project of the DOE Office of Science's Scientific Discovery through Advanced Computing (SciDAC) Program. Created in 2001, the five-year SciDAC program supports a multidisciplinary, multi-institution teamwork approach to developing the algorithms, codes and software to support terascale computing on problems that often can be solved only through advances in scientific computing.

"The SciDAC model has just been amazing. It's changed the way we do science, and I quite honestly feel that for the very first time we can address these scientific problems for what they are rather than whittle them down to something that you can handle. I've never felt better as a computational scientist in my life," says 46-year-old Oak Ridge National Laboratory theoretical astrophysicist Anthony Mezzacappa, who's been modeling supernovae for almost 20 years and is TSI's project manager.

Mezzacappa says that SciDAC has enabled TSI to efficiently tackle problems that require applied mathematics one day, terascale networking the next, and the integration of quantum-level nuclear physics with general relativistic-level astrophysics the next.

And this multi-disciplinary team approach is paying off. Through computational modeling, TSI members — including Steve Bruenn from Florida Atlantic University — have discovered two post-core collapse instabilities that significantly alter how a supernova explodes.

"We discovered that the shock wave itself can become unstable, either aiding or altering the shape of the explosion," says Mezzacappa."Like the SciDAC name says, that was scientific discovery through advanced computing."

ANTHONY MEZZACAPPA

Dr. Anthony "Tony" Mezzacappa is a Distinguished R&D Staff Member and Group Leader for Theoretical Astrophysics in the Physics Division of the Oak Ridge National Laboratory. He is also Adjunct Professor in the Department of Physics and Astronomy at the University of Tennessee. He has been on staff at the Laboratory since 1996 and associated with the University of Tennessee since 1994. He held postdoctoral appointments at the University of Pennsylvania and the University of North Carolina at Chapel Hill and a research faculty position at the University of Tennessee prior to joining the Laboratory staff. He completed his B.S. degree in physics at M.I.T. in 1980 and his Ph.D. in physics at the Center for Relativity at the University of Texas at Austin in 1988. He has worked in the areas of astrophysics and cosmology and specializes in the theory of supernovae. He has been studying supernovae since 1986. In 1999, Tony received a DOE Young Scientist Award from Secretary of Energy Bill Richardson and a Presidential Early Career Award from President Bill Clinton for his supernova work. Tony is now the Principal Investigator of the Department of Energy's TeraScale Supernova Initiative, a multi-year, multi-million-dollar national initiative involving several dozen researchers from a dozen institutions across the U.S.

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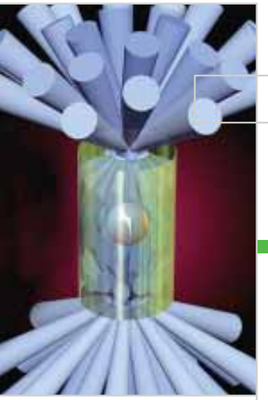
World's Largest Laser System



THE STADIUM-SIZED National Ignition Facility (NIF) currently under construction at the University of California's Lawrence Livermore National Laboratory (LLNL) is the largest laser and optical system ever conceived. When NIF is completed, in 2008, it will be capable of delivering 192 beams of the most energetic ultraviolet light ever generated to targets a few millimeters in diameter, precisely located inside NIF's 10-meter diameter aluminum target chamber.

One of NIF's principal missions is to develop fusion energy gain in the laboratory for the first time, which could lead to a limitless and relatively clean power source. Unlike nuclear fission, which produces electricity in today's atomic power plants by use of, and producing, long-lived radioactive materials such as uranium and plutonium, fusion uses isotopes of the abundant element hydrogen — deuterium and tritium — as fuel, and leaves shorter-lived and less hazardous radioactive by-products.

Nuclear fusion has already been created by use of earlier large laser systems, such as the Nova laser, which was also located at LLNL — but to date, more laser energy has been required to begin the process than can be derived from it. At NIF, on the other hand, the expectation is to produce nuclear fusion outputs that are 10 times larger than the UV laser energy required to initiate the fusion process.

The Lasers

NIF lasers dwarf standard laser systems — each laser beam has a 40 cm by 40 cm cross section. The beams are focused and conditioned by very high quality refractive and diffractive optics to spots, a few tens of microns to a millimeter in diameter, exactly at the center of the target chamber. The immense energy at NIF, up to two million joules of laser light (60 times the energy of the Nova laser), is concentrated into a cubic millimeter, creating conditions of energy density approaching those in the center of stars or exploding nuclear weapons.

Experiments at NIF will produce pressures greater than one billion atmospheres and temperatures of tens of millions of degrees. Under these conditions of high energy density, solid materials can be made to flow like liquids, and intense shocks can be propagated through materials, leading to changes in their crystalline structures or turning them into high temperature plasmas. Materials science and scaled astrophysics experiments are planned to be studied using the National Ignition Facility to reach pressures and temperatures far beyond what is currently available in the laboratory using high explosives, gas guns, and pulsed power systems.

Other experiments at NIF will study the process of nuclear fusion, the same process that powers the sun and stars and gives modern nuclear weapons their immense energy. NIF fusion experiments will implode specially prepared spherical capsules a few millimeters in diameter filled with frozen deuterium and tritium to produce more energy than required to initiate fusion reactions. NIF fusion targets use small cylindrical gold cans surrounding the fusion capsule, also known as hohlraums, to concentrate laser energy and convert it to X-rays that drive the fusion implosion.

At NIF, the targets are mostly vaporized under such conditions; however, there can be remnant debris from parts of the target that need to be mitigated to ensure that NIF's optics meet facility requirements for laser beam quality.

Experiments at NIF will produce pressures greater than one billion atmospheres and temperatures of tens of millions of degrees.

Technicians are shown working on the target alignment system inside NIF's 10-meter diameter target chamber. A similar system is used to insert and accurately position NIF experimental targets. In the background the large circular ports are covered by temporary cover plates that will be replaced with final optics assemblies, including the debris shields, that allow laser light to enter the chamber while protecting the laser optics. Smaller openings are provided for experimental diagnostics. The service port at the bottom of the chamber is normally closed and the target chamber kept under vacuum during operation.

The NIF design places the highest value optics behind two windows, also known as debris shields. The window that will bear the brunt of the debris coming from targets is an inexpensive thin sheet of glass called a disposable debris shield, or DDS. Behind the DDS is a thicker, more robust, main debris shield. To fully characterize how NIF's energetic lasers interact with targets to produce patterns of debris with a wide range of velocities and sizes, computational physicist Alice Koniges and her colleagues at Lawrence Livermore National Laboratory (LLNL) are using some of the world's most powerful computers to run three-dimensional models. Their models are designed to simulate what happens inside some of the most hostile environments imaginable.

It is Koniges' job to determine computationally where the bits of target and related matter that are not vaporized when the lasers fire will end up as they hurdle through the vacuum of the target chamber. Traveling at more than half a mile per second, micron-sized debris that hits one of the 192 debris shields leaves an impact pit that, although still very small, can be up to 10 times the size of the debris particle. These small pits have the effect on subsequent shots of scattering laser light away from the

ALICE KONIGES

Alice Koniges is a senior scientist at the Computation Directorate Center for Applied Scientific Computing at Lawrence Livermore National Laboratory (LLNL). She leads the computational modeling effort to predict the impacts of target shrapnel and debris on the operation of the National Ignition Facility.

Her research interests include Arbitrary Lagrange-Eulerian (ALE) methods for time-dependent partial differential equations, high-performance computing on parallel platforms, computational plasma physics, parallel language performance, and benchmarking. Her current work centers on the ALE-AMR code effort that is based on the SAMRAI Framework.

Alice is the first woman ever to receive a Ph.D. in Applied and Computational Mathematics at Princeton University. She also holds M.S.E. and M.A. degrees from Princeton and a B.A. from the University of California, San Diego.

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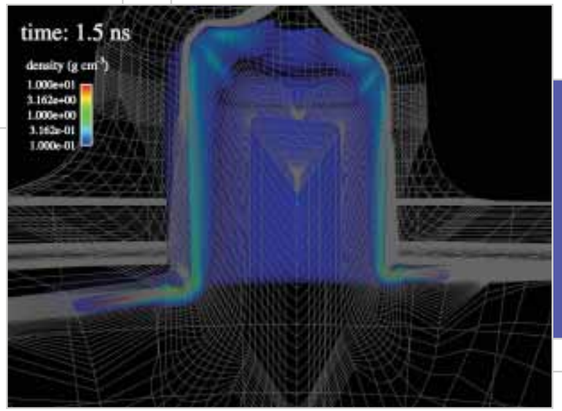


Three-dimensional simulation of the density inside a gold halfraum is shown at a time of 1.5 ns (1 nanosecond is 10^{-9} second). The entrance of the halfraum with surrounding flange is facing downward in this figure. The low-density region on the top is where the 4 laser beams vaporized the back wall of the halfraum.

precise focus, thereby reducing the energy available to drive experiments. Because the debris shields make up one-sixth of the target chamber's inner surface, the effects of target debris are of more than passing interest to NIF scientists, for reasons of both physics and economics.

"If you pepper the debris shield with too many little marks, over time the light will become too diffuse, and then we have to replace the shield," says physicist David Eder, who works with Koniges. Eder is one of many people responsible for approving each NIF firing, of which there have been over 250 to date. He is particularly interested in Koniges' work because he is responsible for predicting and mitigating debris emanating from NIF targets impacting the optics. This can be accomplished by repositioning targets and experimental materials in the chamber, which can alter the trajectory of the debris.

That Is The Question

For each of NIF's applications, numerous types of targets can be used for various experiments. "There are probably 25 different types of targets, and the lasers interact with them differently," said Eder.

This means that each target creates a different pattern of debris, "and we need to know where things go."

That is the question posed to Koniges. Answering it requires extremely complex three-dimensional simulations that became possible only within the past three years, thanks in large measure to the Advanced Simulation and Computing Initiative (ASCI), funded by the U.S. Department of Energy's National Nuclear Security Administration. Earlier two-dimensional simulations could tell physicists what would happen during an experiment but could not track what would happen within the target chamber after a shot.

The complexity of Koniges' modeling challenge is compounded not only by the types of targets, but also by the fact that other materials used in experiments, such as support stalks, can add to the debris generated.

For example, researchers might want to take a pinhole X-ray radiograph of an experiment. To do so, a piece of metal with a small hole drilled in it, much like a *camera obscura*, is placed in front of, and close to, the target. "We then shine X-rays through the hole at the main target we are shooting and record a picture of those X-rays," explains Eder. As the lasers hit the target, that piece of metal "doesn't get completely vaporized." Hence, Koniges' modeling must account for what happens to debris associated with the pinhole as well as that associated with the target itself.

Additionally, her computer simulations must examine events in the target chamber for a considerably longer period of time than the fraction of a second the lasers fire, so that the flight of the debris can be followed. "We want to go 50 to 100 times the few-billionths-of-a-second NIF laser pulse length to follow the material away from the target," says Koniges.

Applying 18th Century Math

The computational processes she applies to her task go under the acronym ALE, for Arbitrary Lagrangian Eulerian, named after the 18th century mathematicians Joseph Lagrange and Leonhard Euler.

"A Lagrange simulation follows the flow of a fluid or plasma. An Eulerian simulation uses a fixed grid and the mass moves through the grid," explains Koniges. "The NIF modeling shifts back and forth between the two methods, depending upon what is appropriate for the flow."

In the course of designing her computer simulations, Koniges also makes use of another advanced modeling technique known as Adaptive Mesh Refinement (AMR). While running simulations of what happens inside the target chamber, Koniges divides her computations into a mesh of mathematical grids, or cells, and examines computationally what is happening inside each of the cells. This enables computations to be broken down into manageable chunks, yet when a great deal of activity is taking place in a few cells and not much is happening elsewhere, it is a waste of computer power to have it focus on all the grids in the mesh equally. AMR enables the computer to focus the majority of its diagnostic power on the grids in which the most action is taking place.

Combining ALE and AMR provides "a whole new mathematical tool set, which makes it interesting, because some of the algorithms are brand new and haven't been used before," says Koniges.

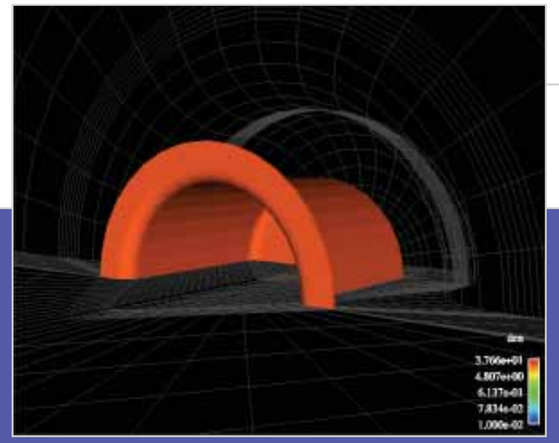
Performing such calculations requires massive computing power, which is just what LLNL has available. "We couldn't do this if we didn't have some of the top computers in the world," says Koniges, who writes her computer codes so that they can operate on a variety of platforms, allowing her to use whatever is available and what she needs for any given simulation. "Sometimes the problems will be slightly more memory intensive and then we will use a computer with a larger memory, and sometimes we'll need more processors with fewer bits of memory," she explains.

LLNL's ASCI White supercomputer, which is among the world's most powerful, is one system Koniges has at her disposal. She also makes use of clusters of parallel computers. "We've got some new, very fast switching and coupling technology that's produced some really nice computing clusters, so I do a lot of the simulation on the clusters," she says.

Currently Koniges is running simulations of what happens when NIF fires at an empty half hohlraum, called a halfraum. She and her colleagues will then move to examining a model hohlraum, with a fusion capsule placed inside.

While NIF's target chamber environment can be characterized as extremely challenging, physicists such as Koniges and Eder are at the forefront of this sophisticated modeling effort to ensure that NIF's availability and performance meet programmatic requirements.

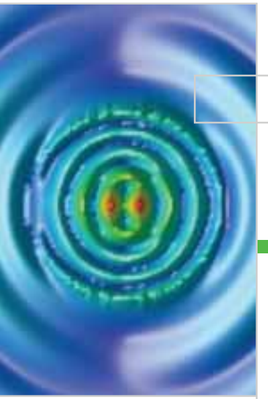
For each of NIF's applications, numerous types of targets can be used for various experiments.



A gold halfraum (an empty half hohlraum) from a 3D simulation is shown with only the outer edge of the mesh visible. The halfraum has a flange that opens outward at the entrance. Such targets are being shot currently on NIF with 4 laser beams striking the back of the halfraum.

By Peter Gwynne

Diverse by Design



>> Accelerator Design
>> Verification & Validation
>> Astrophysics
>> Laser Science
>> Applied Mathematics
>> Infrastructure Analysis
>> Environmental Science
>> Transportation Engineering

LOCATED ON LONG ISLAND, the Brookhaven National Laboratory has a proud record of achievement in areas as diverse as the discovery of new fundamental particles; the creation of L-dopa, a drug used to treat Parkinson's disease; and the development of magnetically levitated trains. Much of its research involves actual experimentation.

Some of the experiments performed at Brookhaven are so costly and complex that Brookhaven's scientists choose to rely, at least in part, on computer simulations provided by the laboratory's Center for Data Intensive Computing (CDIC).

The center has wide-ranging responsibilities. "Brookhaven is a multipurpose lab and has a lot of different needs for computational science; one of our goals is to represent those needs," says center director James Glimm. "Another goal is to do first rate research, which is also diverse. We're involved with accelerators, fluid dynamics, nanoscience, and biology, as well as the design of high performance computers in terms of understanding how they work and how algorithms get ported into them. We try to cover the main bases that are important for Brookhaven as well as we are able to."

In doing so, the center acts as a significant adjunct to Brookhaven's researchers. It merges its expertise in simulation with the researchers' knowledge of their own fields to create a synergistic relationship. "People who know the work don't necessarily have the computational understanding," Glimm says. "We provide that understanding."

Two Projects

Two projects illustrate CDIC's breadth of expertise. One explores the feasibility of a new type of target for producing intense beams of the elementary particles known as muons, which have the same electric charge as conventional electrons but about 200 times the mass. The other simulates the activity of a vertical cavity surface emitting laser (VCSEL), a device that has a wide range of practical applications in optics. Both efforts have already played a role in gaining a fundamental understanding of the nature and behavior of matter. And the solutions of both have already demonstrated utility beyond their original *raison d' être.*

Simulation of the creation of muons by firing beams of high-energy protons at small jets of liquid mercury in strong magnetic fields promises to lead to a working muon collider — a new, more efficient type of particle accelerator that will delve deeply into the nature of matter by causing intense beams of muons to smash into each other. "The muon collider is a very new idea; it didn't exist a few years ago," says Roman Samulyak, a research associate at CDIC. "And liquid targets are the future for the majority of advanced particle accelerators." In addition, Samulyak continues, "Liquid mercury is the choice of target for the Spallation Neutron Source," a device that creates intense beams of neutrons for both fundamental science and industrial applications that range from materials science — in the structural analysis of solids — to biology — analyzing the shape and structure of proteins. He is also carrying out simulations of targets made of liquid lithium.

The overall goal of this work fulfills the Department of Energy's mission of studying fundamental physics at extreme conditions. "The accelerators measure the behavior of particles at very high energies," Glimm explains. "They cannot be built without adequate target design."

[The center] merges its expertise in simulation with the researchers' knowledge of their own fields to create a synergistic relationship.

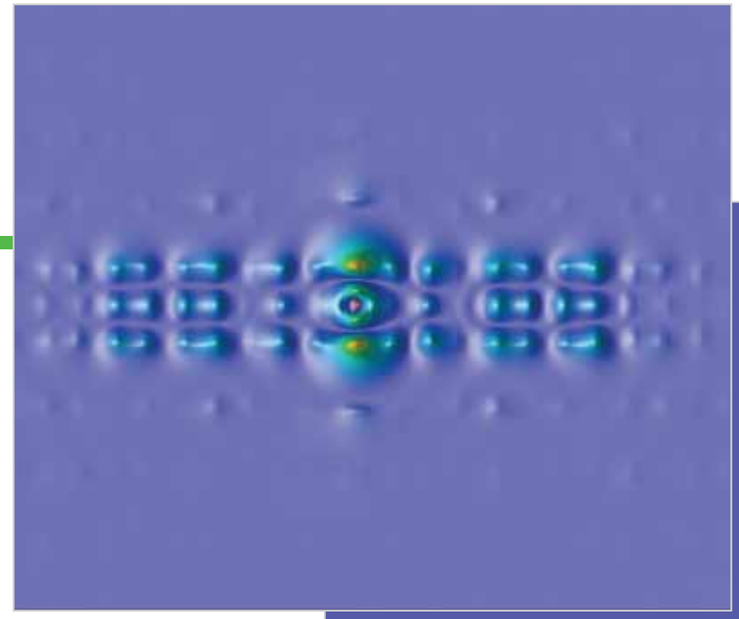
Electromagnetic Equation Solver

The work on VCSELs focuses on a photonic crystal VCSEL that has holes of different depths and diameters etched in the side of the crystal to provide a wave guiding effect. "One aim," says Nick D'Imperio, a physics associate at CDIC who oversees the research, "is to increase the power output of VCSEL lasers." The research quickly expanded beyond that single goal. "We realized that it would be a simple matter to make the code adaptable to solving general problems," D'Imperio says. "We incorporated our code into particle tracking simulations also developed here at Brookhaven, which I believe has not been done before."

The key to CDIC's work is the use of computer codes that solve Maxwell's equations, a group of four powerful mathematical relationships set out by Scottish physicist James Clerk Maxwell in the mid-1860s that associate the behavior of electric and magnetic fields at single points in space with changes in those fields at other points in the immediate vicinity.

Maxwell solvers are relatively common in the public and private sectors. However, Glimm says, "Those that are public are not very good, and those that are strong are expensive." D'Imperio echoes that thought. "Available simulations have a lot of commercial value," he says. "You'll see a lot or proprietary algorithms out there." But in addition to high cost, the commercial algorithms don't fully meet CDIC's needs. "So we decided we needed a code that could scale to hundreds, and perhaps thousands, of processors," D'Imperio says.

The code that D'Imperio's group designed for work on VCSELs, says Glimm, "already has rather nice scientific capabilities. It's three-dimensional, and it gives the best version of boundary conditions." Similarly, the code that Samulyak's team designed for simulating hydrodynamic and magnetohydrodynamic processes in mercury targets has specific advantages over others. "Our code has been somewhat unique in getting good agreement with experiment," Glimm says.



Longitudinal slice showing the electric field energy excited by an electric dipole located in the defect layer of the VCSEL. Energy confinement due to the photonic crystal is very high and single mode excitation is evident.

From Simulation to Experiment

In contrast to the usual sequence, Samulyak's simulations preceded experimentation on the use of liquid mercury targets to create muons. "It's a very challenging problem of solving partial differential equations in varying geometries. When we started to work on the project we didn't have any experiments," he recalls. "Theoretically we were looking for an optimal design to solve the problem." Indeed, he points out, "Our main practical goal

JAMES GLIMM

James Glimm is Director of the Center for Data Intensive Computing at Brookhaven National Laboratory (BNL) and Chair of the Department of Applied Mathematics and Statistics at the State University of New York at Stony Brook. He has previously held faculty positions at New York University, Rockefeller University and MIT.

He is a member of the National Academy of Sciences and a recipient of the Steele prize of the American Mathematical Society, the Dannie Heinemann prize of the American Physical Society, the New York Academy of Sciences award in Mathematical and Physical Sciences, Guggenheim fellowships, and a special commendation from the Society for Industrial and Applied Mathematics for leadership in Industrial Mathematics.

He is a member of the External Advisory Committee for the Dynamic Testing Division at Los Alamos National Laboratory and chair of the Advisory Committee of the Weapons and Material Science Directorate at the Army Research Laboratory. His research interests include computation and modeling for turbulent and chaotic flows, mathematical theory of conservation laws, stochastic methods, modeling of elastic-plastic deformation, methods for the quantification of uncertainty, and the application of mathematical methods to industrial problems.

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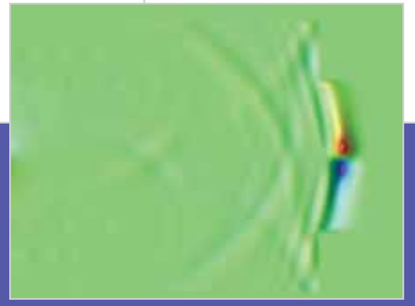


The following three images are of a gaussian bunch of particles passing through a RF cavity. The images show the Y component of the electric field. The wake caused by the bunch's interaction with the cavity can be clearly seen.

Beam 1: *The bunch is just passing the junction where the pipe is attached to the cavity.*

Beam 2: *The bunch is at the midpoint of the cavity.*

Beam 3: *The bunch is exiting the cavity and has entered the trailing pipe.*

is to understand the behavior of the target and ultimately to be able to replace a real experiment with a simulation."

The concept involves firing a series of liquid mercury jets, each about one centimeter in diameter and 30 centimeters long, into a 20 Tesla magnetic field at a speed of 30 to 35 meters per second. As each jet reaches the center of the magnetic field, it encounters a pulse of protons. The collision creates a beam of muons, but not without some difficulty. "The particles are moving very fast and you're depositing huge amounts of energy, so that the targets suffer heavy damage," Glimm explains. "The question is whether you can get several bunches of protons onto the mercury target without its evaporating or going into droplets."

Samulyak's early simulations revealed potential problems associated with that simple concept. For example, strong waves in the target caused by the impact of the protons cause surface instabilities that quickly break up the target. On the other hand, the simulations also showed that the strong magnetic field tends to stabilize some expected instabilities in the jet of liquid mercury. Initial experiments at Brookhaven agreed with those findings. "Our next series of preparatory experiments is planned at CERN [the European Center for Nuclear Research in Geneva, Switzerland]," Samulyak says. "And the real experiments will start in 2006."

The Importance of Collaboration

The work with CERN scientists, which includes target studies for the muon collider, illustrates the collegial nature of CDIC's work. "I'm also collaborating with people at the Oak Ridge National Laboratory who work on a liquid mercury target for the Spallation Neutron Source," Samulyak says. "And I'm planning to work with scientists at the University of Michigan's superconducting laboratory."

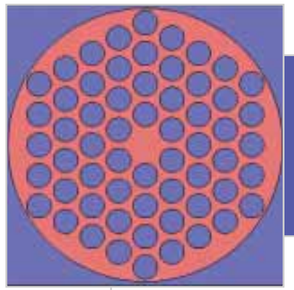
Collaboration also features strongly in CDIC's simulations of crystals for VCSELs. "This is an active collaboration with two professors, Joe Haus and Andrew Sarangin at the University of Dayton," says D'Imperio, who is studying for a Master's degree in addition to performing his work at Brookhaven.

What value does collaboration have generally in simulation studies? "Our work would be totally impossible without collaboration with other groups," Glimm asserts. "Experiments are crucial to complement simulations, and this calls for more interaction. Collaboration is basically why we're here and why it's fun to be here."

Equally important to CDIC's success is the availability of high performance computing on and close to the Brookhaven campus. "We have a cluster of computers that are part of our unit," Glimm says. "We also have very good computer facilities at the nearby State University of New York at Stony Brook," where Glimm chairs the department of applied mathematics. D'Imperio's group, for example, carries out its simulations on Brookhaven's Galaxy cluster, a set of computers running the Linux operating system.

CDIC will soon acquire a machine of its own with significantly greater computing power. Called the QCDOC, it will enable computer scientists to simulate problems in quantum chromodynamics, one of the fundamental approaches that underlie current understanding of elementary particles. "The machine will have 20,000 different processors," Glimm says. "You would never have that in a university." Like many of the other tools and technologies in CDIC's locker, the new machine will have application beyond the immediate issue for which the center has acquired it. "We looked at it and found more or less to our surprise that it was useful for studying biological problems such as the Coulomb force," Glimm says.

Glimm himself, who started work on computer simulations during the Arab oil embargo in 1973 by modifying a theorem of his for use in computational methods, recently received a significant award for his contributions: the Presidential Medal of Science. Samulyak and D'Imperio, meanwhile, are working on their own forms of recognition, by publishing scientific papers on their research that will inevitably be cited by future scientists working on the fundamentals of matter and the applications of photonics.



Transverse slice through the defect layer of the VCSEL showing the triangular lattice of the photonic crystal with the central defect region.

PASSIVE & PROACTIVE

>> ***Finding problems to solve at the Center for Data Intensive Computing demands a combination of passive and proactive approaches. Research teams at the Brookhaven National Laboratory frequently ask CDIC scientists for help simulating the solutions of problems that are too expensive or too complicated to attack effectively by using traditional experimentation. But the Center also takes an entrepreneurial attitude to new projects. "If we waited for walk-ins, we would be a failure," says CDIC director James Glimm. "So we go out and actively seek problems. That's part of the fun."***

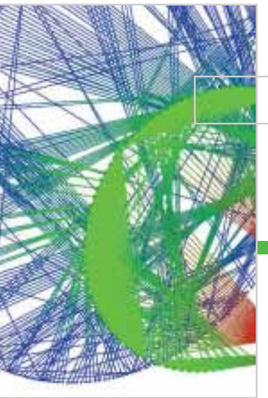
That proactive approach benefits from the speed with which computer scientists can set up simulations. "The time we need to get into a new subject is not that big," Glimm explains. "We can go to a person, propose a project, and start work on it quickly."

The center's skills have particular value for scientific teams inexperienced in computing and simulation techniques. For example, Glimm says, "We have biologists across the hall who need all the help they can get in their research, but they're not trained in computational methods. We don't have prior experience in biology, but we can quickly gain enough understanding." That leads to a win-win situation: the biologists can use the simulations to advance their research, while CDIC's computer scientists gain valuable insights into a new field that will improve their ability to help their scientific colleagues.

As an example of that interaction, Glimm recalls that a graduate student from Harvard University working on a summer internship at CDIC began work on a problem of interest to biologists. "Then a graduate student in chemistry continued the work, running the simulation codes," he says. "In the process, we learned how the biological systems worked and were able to build our own codes to run on modern computers. So computer architecture and advanced algorithms came into the picture, even though they were off the scope of our original focus."

Modeling Municipal Movements

By Peter Gwynne



A SIMULATION SYSTEM developed at the Los Alamos National Laboratory permits planners to model the impact of proposed changes in infrastructure on the populations of cities and regions.

When they try to determine whether planned traffic improvements such as widening a highway lane or erecting a new bridge will actually work, municipal authorities face a significant roadblock. "It's not feasible to do experiments on a real system to test the suggested changes," says James Smith, a technical staff member of the Basic and Applied Simulation Science group in the Los Alamos National Laboratory's Computer and Computational Science Division.

In the past, authorities made do with a partial solution to that problem: they hired consultants to study the plans on the basis of historical information. Now, however, an approach developed by the Los Alamos group offers a much more rational way to predict the effect of specific changes to a city's — or a region's — infrastructure. The Transportation Analysis and Simulation System (TRANSIMS) is an integrated system of forecasting models intended to give transportation planners accurate and complete information on every facet of activity that affects the movement of traffic and people in areas that range in size from a small village to a large metropolitan region.

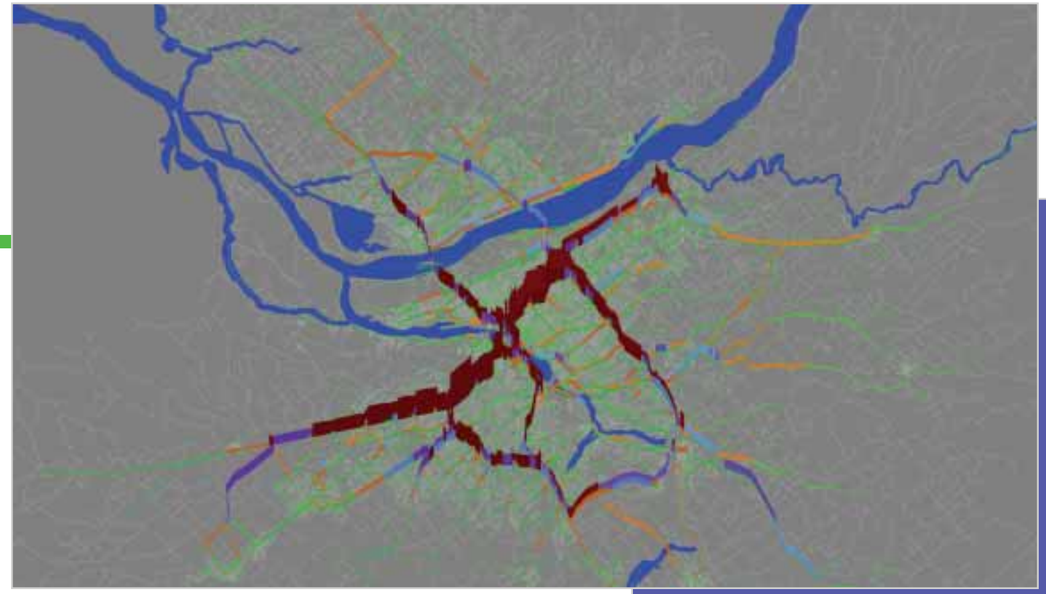
The system is designed to provide reliable, detailed information on the impact of planned infrastructure improvements or changes on traffic patterns, congestion, and even air pollution. "With simulation, you can make informed decisions," Smith explains. "Simulation essentially gives you an experimental platform for the planning."

TRANSIMS consists of a group of computer models that provide a complete representation of the individuals who live in a region, along with their activities and the region's transportation infrastructure. The models simulate the movement of people around that transportation network, taking note of their mode of travel, such as buses or cars, on a second-to-second basis. Among other things, interactions of vehicles shown by the models permit analysts to judge the efficiency of the transportation network and to estimate the extent of emissions from vehicles into the local atmosphere. And because TRANSIMS is a group of modeling tools, planners can use it to evaluate how proposals for changing traffic patterns will affect a region as a whole and their impact on individual segments of its population.

Demonstration Projects

Having originated about a dozen years ago, TRANSIMS initially proved its value through demonstrations in Albuquerque, New Mexico, and a segment of Dallas. "Then we did Portland, Oregon, to show that we could do a whole city with all modes of transport," Smith says. More recently, he continues, "we have extended our models to estimate the social network of who is doing what with whom with respect to time in a community."

Those successes have caused significant changes in attitude toward TRANSIMS. "Most of the transportation community didn't really think it was possible when we started," Smith recalls. "There was great skepticism. It was a hard fight at the beginning for us and our sponsors." Now, the community has largely accepted the approach. "If you go to a transportation conference, you find that many people are taking similar approaches," Smith says. Transport experts are licensing the system from IBM Business Consulting Services, which has a commercial agreement with Los Alamos.



Net simulated traffic volume on all roads in Portland at a particular time of day. Tall red bars usually indicate the high-traffic freeways and green the less used arterials. Local streets cannot be seen in this visualization.

The TRANSIMS approach doesn't apply simply to traffic. Scientists have also used the system to model air quality in metropolitan areas, and the Los Alamos team has adapted its technology to create EpiSims, a system that can follow the spread of disease through a population. Public health authorities have already used EpiSims to help determine the most effective response to outbreaks of infectious diseases. In these and other fields, the Los Alamos team publishes between 20 and 30 papers on its research each year in refereed journals. And academic institutions such as the University of New Mexico and Virginia Tech now include this type of simulation mathematics in their courses, an astonishing fact considering that it usually takes 50 years to get new mathematics into the curricula.

Not surprisingly, research on TRANSIMS demands expertise far beyond computer skills and knowledge of traffic patterns. "We have people from many different fields," Smith says. "They include chemists, physicists, engineers, mathematicians, public policy people, and epidemiologists. Everyone works on the problem from their own discipline's point of view."

Development of the system has involved federal and local agencies beyond the Department of Energy, which oversees Los Alamos. "We're experts in computer science, mathematics, and modeling," Smith explains. "We couldn't have done TRANSIMS without a collaboration with the Department of Transportation. We have also collaborated with academic researchers, the Portland Metropolitan

The Transportation Analysis and Simulation System (TRANSIMS) is an integrated system of forecasting models intended to give transportation planners accurate and complete information on every facet of activity that affects the movement of traffic and people in areas that range in size from a small village to a large metropolitan region.

COLLABORATORS

James P. Smith is a technical staff member in the Basic and Applied Simulation Science Group of the Computing and Computational Sciences Division at Los Alamos National Laboratory. His principal interest is in high performance computing applied to modeling, simulation and analysis of socio-technical systems. His current research applies to national infrastructure, especially telecommunication/computing, public health, and transportation. He has scientific experience in high performance computing and parallel processing applied to large-scale microscopic simulations, including original software design and debugging of very large, evolving systems of inter-operable computational systems, and efficient analysis and synthesis of massive data produced by multi-scale complex environments. He has publications in biophysics, analytic finance, education, space plasma physics and computer science, and is a co-inventor on the TRANSIMS patent. He has a Ph.D. from the University of Texas at Austin.

Before retiring earlier this year, **Christopher L. Barrett** was leader of the Basic and Applied Simulation Science Group of the Computing and Computational Sciences Division at Los Alamos National Laboratory. He has scientific experience in simulation, scientific computation, algorithm theory and development, system science and control, engineering science, bio-systems analysis, decision science, cognitive human factors, testing and training. His achievements include development of large-scale, high performance simulation systems and development of a distributed computing approach for detailed simulation-based study of mobile, packet-switched digital communications systems. Barrett has an M.S. and Ph.D. in Bio-information Systems from California Institute of Technology. He has received three Distinguished Service Awards from Los Alamos National Laboratory, one from the Alliance for Transportation Research, one from the Royal Institute of Technology, Stockholm, and one from Artificial Life and Robotics, Oita University, Japan.

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Planning Office, and the Environmental Protection Agency. And for EpiSims we have collaborated with the Department of Health and Human Services." Most recently, the team has worked on improvements to its models as part of an infrastructure project in homeland security.

A "Socio-technical System"

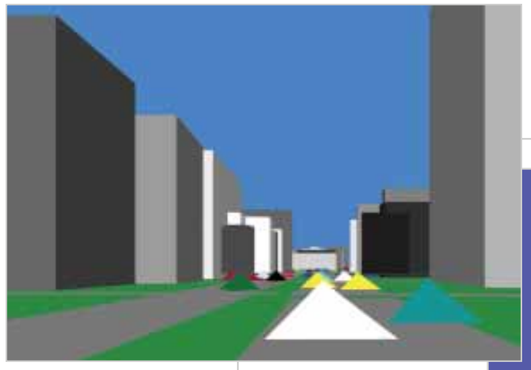
Technically, TRANSIMS simulates a "socio-technical system," a term indicating a system that is affected by a variety of influences. That designation recognizes that relationships between cause and effect don't always work out as expected.

The modeling involves more than specifically physical phenomena. "Unlike physical systems, socio-technical systems are affected not only by physical laws but also by human behavior, regulatory agencies, and government and private enterprise," Smith's colleague Christopher Barrett and his collaborators write in a recent issue of *SIAM News.* "The situation of such systems thus presents novel challenges to researchers. Urban transportation systems constitute a canonical example of the types and levels of interactions that characterize these systems: traffic rules in distant parts of a city can have an important bearing on traffic congestion downtown, and seemingly 'reasonable' strategies, such as adding a new road somewhere, might actually worsen the congestion."

TRANSIMS takes account of the fact that individuals basically determine traffic patterns. When a particular trip takes too long, for example, people find other routes, take their automobiles instead of buses or vice versa, travel at different times, or forgo the trip entirely.

The simulations are based on a mathematical and computational theory of socio-technical simulations and combined with the Los Alamos team's own methods for designing and analyzing large dynamic networks and efficient techniques for compressing and regenerating data. The team developed a mathematical approach known as Sequential Dynamical Systems that captures the core features of computer simulations and permits its users to analyze them formally. "We've come up with mathematical generalizations of simulations with Sequential Dynamical Systems," Smith explains. "The formal mathematics makes us think the right way when we design our simulations."

Application of the approach creates a suite of simulation tools, called the Urban Infrastructure Suite, that models every facet of an urban environment, from buildings and transport systems to telecommunications and water distribution. "As a result," Barrett writes, "the simulations are capable of representing, in extreme detail, millions to tens of millions of interacting agents." Indeed, detailed socio-technical simulations on that scale don't exist anywhere beyond Los Alamos.



A 3D visualization of the results of the high-traffic microsimulation, from the point of view of a traveler riding in one of the vehicles.

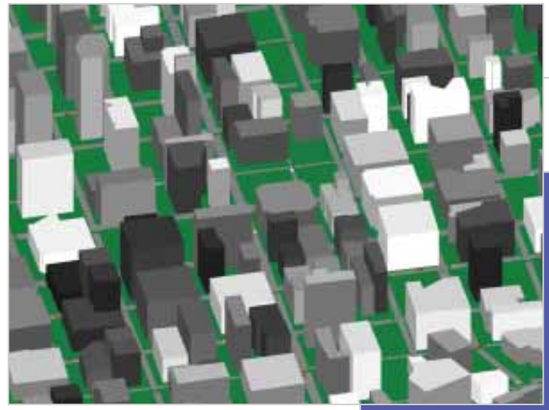
Power of the Simulations

The application of TRANSIMS to the city of Portland illustrates the power of the simulation technique. The system can represent every member of the city's roughly 1.6 million population on a second-by-second basis at a resolution of several meters. The system also models the approximately 8 million trips that Portlanders take every day.

To satisfy their sponsors and the computer scientists who develop them, the simulations must fulfill strict requirements. They must consider the interactions of all vehicles on the urban area's roads; know the locations, speeds, and accelerations of all those vehicles; understand the impact of a multimodal transportation system that includes cars, buses, and other vehicles; and realize the purpose of each trip every person takes in the area and the individual travelers' demographics. In addition, the simulations must achieve all those goals within the constraints of the existing urban environment and have the ability to model adaptations of individuals' behavior in response to changes in the urban infrastructure, such as the opening of new roads, office buildings, or shopping malls.

To achieve those goals, the TRANSIMS team needs significant amounts of computing power. "You need millions to billions of agents," Smith comments, adding dryly that "You can't do it on a laptop." The Los Alamos group has the advantage of access to powerful supercomputers at the national laboratory. The scientists needed that access because the Department of Transportation required a simulation system that could work in any metropolitan region and could apply even to a huge metropolis such as Chicago.

Supercomputers aren't essential, however. "The minimum you would need for a moderate-sized city is a small Linux cluster that does about 100 billion operations per second," Smith says. "These are accessible to any university."



Another 3D visualization from above the road network, also showing the actual buildings, cars and roads.

Equally important is the ability to store the huge amounts of data involved in TRANSIMS simulations. The Los Alamos group routinely carries out research on efficient storage and — because the simulations involve far too much information for all of it to be stored at any one time — regeneration of the dynamical information.

A Vital National Requirement

Why should a national laboratory devoted to ensuring national security involve itself in simulating people's movements in cities? "A detailed representation of the various components of an urban infrastructure is a vital national requirement that motivates rigorous simulation methods," states the Computational Science Division's website. Smith puts it in a slightly different way. "The national laboratories carry out the world's greatest science to protect America," he says. "We intend to remain the preferred lab for science and development."

Smith himself illustrates the variety of experiences on which the TRANSIMS team can call. He started out as a biophysicist, worked on theoretical plasma physics, and entertained a job offer from NASA before opting to work at Los Alamos five years ago. "I've been in simulation science ever since," he says.

SETTING UP THE SIMULATION

>> ***The precision of modeling undertaken by TRANSIMS relies heavily on obtaining a realistic representation of the mobility of individuals in a town or region. That requires researchers to assemble detailed outlines of streets, highways, signals, and signs, as well as transit information and locations such as parking lots where activities take place.***

Pulling together all that information isn't easy. Because privacy issues prevent the Census Bureau from releasing full records of people in any location, researchers must create synthetic populations that match real ones, based on anonymous samples from the Bureau. Researchers must then generate a set of activities for every person in the synthetic population. To do so, they rely on surveys of individuals' movements routinely undertaken by most metropolitan planning offices, and data on land use and travel times between specific locations by various modes of transport, also readily available.

The information permits the team to build up an accurate picture of what each member of its synthetic population is doing and where he or she is doing it — taking a bus to work, shopping at the corner grocery, or walking back from a local restaurant, for example — at any time of the day. Recognizing that families are more basic units than individuals, the simulation team translates its findings into activities by households. By choosing random groups of households, the team can put together a network that indicates the travel patterns of everyone in the synthetic population. The result is a realistic social network that forms the underpinning for TRANSIMS modeling.

By Karyn Hede

Moving Mesh

>> Accelerator Design
>> Verification & Validation
>> Astrophysics
>> Laser Science
>> Applied Mathematics
>> Infrastructure Analysis
>> **Environmental Science**
>> Transportation Engineering

THE TRIANGLE, a shape so simple that even a three-year-old child can recognize one instantly, has nonetheless engaged mathematicians since antiquity. For Harold Trease, a computational physicist at the Department of Energy's Pacific Northwest National Laboratory (PNNL), the triangle forms the basis for a three-dimensional mesh generation program that has taken modeling of complex physical and biological systems to a new level.

"The only element that will map a complex surface is a triangle," says Trease. "It can faithfully represent any shape in three dimensions. The mathematics we use is high school-level geometry. If you think about it in terms of conservation of mass and momentum it becomes a simple problem. Forces push on one area of the triangle and it reacts."

When explained this way, creating a responsive three-dimensional virtual object sounds elementary. But the fact is that Trease is one of only a handful of computational physicists worldwide who have worked out how to start with a flat image and reconstruct a three-dimensional representation of that image that can then react realistically to simulated forces. His program, called NWGrid, contains more than a million lines of code developed over 25 years and is designed to run on a massively parallel computer network. Its purpose is to enable scientists to model the most complex interactions of solids and liquids moving at high speed.

"The mesh is not a mesh that just sits there, it moves around," he says. "In all the problems we do, there is this aspect of moving geometry, and you have to have numerics that can track those movements and yet maintain the surface geometry. This is a fairly subtle aspect that makes NWGrid unique and that you could never do outside of a national laboratory, because of the computational power required."

Trease originally developed the code, called X3D, at Los Alamos National Laboratory to simulate high speed impacts and explosions, but it turned out that the dynamic nature of the mesh makes it perfect for simulating complex biological systems. He arrived at PNNL in 2000, code in hand, ready to convert X3D from a computational physics code to a biophysics/bioengineering code.

"One of the unique things about doing large-scale code development within the DOE, compared to other places, is that I get to take a long-term view of code development to continually evolve the code to keep it current with modern programming and hardware paradigms," says Trease. "Biology has some of the same sort of features — the interaction of solid and fluid materials and how they respond to each other — that we were trying to characterize in a physical system. NWGrid allows you to naturally capture the multiscale features of biological problems that are otherwise tough to represent."

Fish and Flocs

PNNL hydrologist Marshall Richmond has teamed with Trease to learn how to modify the operations and physical structure of dams to maximize the survival of salmon and other fish. Richmond is part of a team of scientists studying spillway and turbine passage routes for migrating salmon at several dams on the Columbia River in Washington state with an eye to understanding the physical forces that contribute to fish mortality. The scientists are using NWGrid to predict the stress levels that fish might experience based on different water jet speeds used in guiding the fish through the dam.

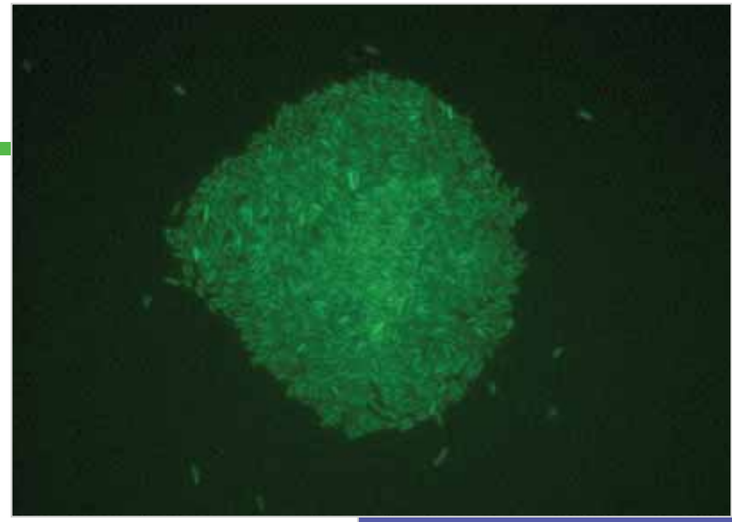
The mesh is not a mesh that just sits there, it moves around…

Trease knew that he could effectively model the force of the water jet and the fluid flow, but modeling a swimming salmon was a challenge. In his first effort, the fish look wooden, like fishing lures bobbing in a trout stream. Once he was satisfied that the simulation effectively modeled the forces on a "solid" fish, he began adding "fish characteristics," giving the fish a flexibility and simulating a swimming motion.

The research team then added data obtained in real-world experiments in which an electronic sensor monitored pressure and acceleration as it traveled through an actual dam.

Finally, they began simulating the actual forces experienced by a flexible swimming fish. While the project is still in its early stages, the scientists are hopeful that by comparing data obtained in experimental systems to the computer simulations, they will gain a better understanding of the conditions that may be responsible for fish injury and be able to make recommendations for improvements.

"The great thing about this model is that once we are sure the math is correct, we can compare our simulation to the experimental system and see how closely it matches the data," says Trease. He emphasizes that what makes NWGrid so useful is its ability to model at multiple scales. So while he can model a fish swimming, he can just as easily model the behavior of microbes, both individually and by the millions.



This figure is one confocal image slice from a three-dimensional stack of confocal images. This image shows a floc of Shewanella microbial cells that have aggregated into a three-dimensional structure, consisting of thousands of individuals, due to a hostile environment created by an increase in the substrate oxygen concentration.

Trease's mesh is a key element in an ambitious project whose goal is nothing less than simulating a living cell complete with all its genetic and biochemical complexity. PNNL microbiologists Jim Fredrickson and Yuri Gorby are teaming with collaborators at Argonne and Oak Ridge National Laboratories, the University of Southern California, Michigan State University, and the biomedical research center BIATECH of Bothell, WA., to investigate just how a common sediment bacterium called *Shewanella oneidensis* is able to metabolize heavy metals, such as uranium.

"The project is directly relevant to DOE's mission, because *Shewanella* is efficient at metal reduction and immobilization of contaminants," says Fredrickson, coordinator of the DOE-sponsored *Shewanella* federation. "*Shewanella* is typically found in sediments and bodies of water, in transition areas of the environment where oxygen is low or absent. It can use a range of metals for respiration in place of oxygen, gain energy from that, and compete with other organisms in that environment."

HAROLD TREASE

Harold Trease is a Senior Research Scientist in the Computational Science and Mathematical Division within the Fundamental Science Directorate at Pacific Northwest National Laboratory (PNNL). He is currently leading the P3D Code Development Project at PNNL. P3D is a computational physics simulation framework that includes three-dimensional, unstructured, hybrid, parallel, time-dependent mesh generation, setup, and computational solvers.

P3D is being developed as part of the DOE's SciDAC TSTT (Terascale Simulation Tools and Technologies) Center, where Harold is the PNNL PI. The two codes that form the basis of the P3D framework are NWGrid and NWPhys. NWGrid is a mesh generation code system and NWPhys is a discretization/solver code system. Harold is applying his high-performance, parallel computing capabilities in several areas, such as: computational biology (e.g. the imaging, modeling and simulation of microbial cell physiology/kinetics/dynamics, virtual organs, and virtual humans), engineering simulations, atmospheric circulation simulations, and subsurface flow simulations.

His principal research interests are in the development and application of parallel high-performance, three-dimensional, discrete algorithms applied to the coupling of fluid dynamics, structural mechanics, fluid/structure interaction, reaction/diffusion, transport algorithms, and MHD. Besides the NWGrid/NWPhys core codes, the development of the computation simulation framework involves the design, implementation and integration of parallel mesh generation, quantitative image processing tools, user interfaces, graphical debugging/display tools, parallel communication libraries, database tools, and configuration management.

Harold received his Ph.D. and M.S. in nuclear engineering from the University of Illinois at Urbana-Champaign and his B.S. in mathematics and physics from the University of Nebraska at Kearney.

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The project's goal is to understand all of the biological processes of the microbe with an eye to capturing and controlling its ability to sequester toxic metals in the environment. Part of the Department of Energy's Genomics: Genomes to Life Program, the project will combine whole-genome DNA microarrays, mass spectroscopy, and more traditional genetic and physiology studies to develop a detailed understanding of the genetic and biochemical pathways of the cell under various environmental conditions. The entire *Shewanella* genome has been sequenced and scientists are currently working to sequence several slightly different strains of *Shewanella* to see if there are significant differences among them. With this information in hand, Trease will create a computational model to predict the organism's behavior as environmental conditions change.

"We are trying to build a mathematical model of the microbes starting with the genome," he says. "If we can get a mathematical model of a single organism based on a series of metabolic pathways then we can simulate how a group of organisms interact in a given environment."

As a first step, Trease has developed a model of the behavior of the organisms, which prefer a low-oxygen environment, when they are exposed to higher levels of oxygen. Biologists had observed that when the microbes are grown in an aerobic oxygen-rich environment they grow hair-like appendages that stick together like Velcro® and cluster in groups called flocs or aggregates.

Trease created a computer model of the oxygen gradient in these flocs and determined that in the center of the flocs there isn't any oxygen. It is thought that the microbes are essentially creating the flocs to protect themselves from the high oxygen environment.

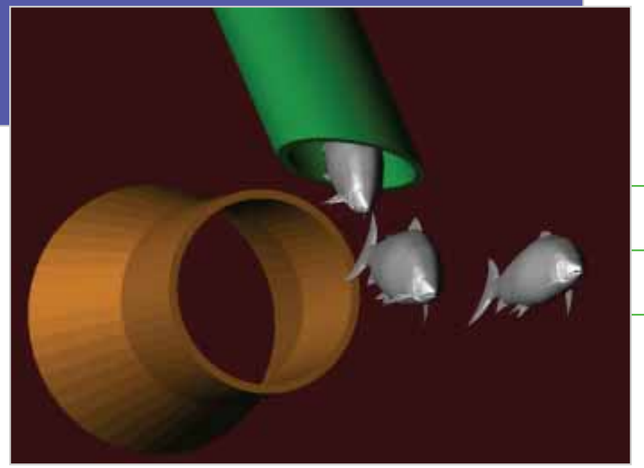
"What he really is doing is developing 3D mesh models of the organism and then mapping various types of functions onto that physical model," says Fredrickson. "From the genome sequence we can gain insights to start to build actual biochemical reactions into the model and have taken the first steps toward doing this. A lot of the modeling done right now has to do with physical control and diffusion of nutrients, but we hope to link their metabolism to changes in the environment so we can really get down to realistically how they work."

We are trying to build a mathematical model of the microbes starting with the genome…

Linking Biology with Computers

In summer 2004, DOE CSGF fellow Amoolya Singh, a graduate student at the University of California, Berkeley, will provide a link between the computational science and experimental biology components of the project when she puts together a series of microarrays designed to tease out the genetic pathways of *Shewanella*. The scientists hope that with this information in hand they will be able to create a computer code that utilizes the organism's genetic code and can be combined with Trease's mesh to approximate a virtual *Shewanella* cell or group of cells.

"Biologists are pretty new to computational modeling," says Trease. "They often don't know what virtual models can do for them. As a community, they haven't been involved in predictive modeling and that's what we are trying to do for them. They can measure some of the details of these metabolic pathways, but they will never measure them all. You just can't do it. And that means somebody has got to come in and fill in these holes. That's where the simulation comes in. In the next couple of years, they are really going to see just what we can do for them. It's a great collaboration."



This figure shows the computation geometry and mesh of three fish being injected into a turbulent water jet. This virtual experiment, which is patterned after the real world experiment, is used to validate the calculated stress field that the fish would be subjected to as they interact with the water jet.

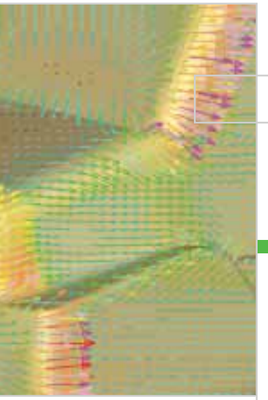
THREE-DIMENSIONAL MESH

>> ***In computational physics experiments, mesh generation is the first step in any calculation. The importance of the mesh to solving the problem can't be overestimated. If the mesh doesn't work, the experiment doesn't work.***

PNNL's Harold Trease designed NWGrid as what is called an "unstructured Delaunay mesh." Basically, it connects points that define object boundaries in a series of triangles called elements. Some areas of the mesh contain fewer points and larger triangles, while other areas that require finer calculation have more finely interwoven meshes. The principle of the mesh structure was derived almost 100 years ago, but its application to computational physics is still a work in progress. Many programmers have created two-dimensional versions of a Delaunay mesh generator, but Trease has taken the idea into three dimensions, something few others have attempted. In fact, many computational physicists still consider three-dimensional mesh generation a "grand challenge" in the field. But NWGrid integrates automated mesh generation, time-dependent adaptivity, applied mathematics, and numerical analysis designed to run on massively parallel computers. NWGrid has already proved itself in calculating fluid-solid interactions, particle transport, biochemical reactions, and aerosol transport. Now it is ready to take on a true grand challenge: simulating life itself.

By Alan S. Brown

Against the Wind



CLASS 8 TRACTOR-TRAILERS are the dreadnoughts of the highway. Hurtling along at 70 miles per hour and weighing up to 40 tons, their wake creates enough turbulence to shake small cars as they pass. Yet at cruising speed, they use only a small fraction of their energy to haul cargo. They expend the rest — 60% for a fully loaded vehicle, 70% when empty — fighting aerodynamic drag.

Parasitic drag, the energy lost pushing through air, accounts for most of the fuel used on long-distance truck trips, says David Weber, Director of New Program Development, Engineering Research, at Argonne National Laboratory in Illinois. If Weber and fellow researchers David Pointer and Tanju Sofu can help truck manufacturers make even modest improvements in drag, they could save the nation billions in fuel costs.

Those modest improvements have been hard to realize using the truck industry's traditional and expensive trial-and-error approach to aerodynamic design. This may be about to change. The Argonne team is developing supercomputing modeling practices that could allow even moderately sized truck makers to switch to faster, less expensive computerized aerodynamic testing techniques. The results could begin to change the appearance of trucks on the road within a few short years.

It's a Drag

Aerodynamic drag, or resistance to movement through air, is measured as drag coefficient (C_D). A typical tractor-trailer's C_D is 0.6. This is less than a bicycle's (0.9) but more than the family sedan's (0.5) or a typical sports car's (0.2 to 0.3). Many engineers believe radical redesigns could halve tractor-trailer C_D to 0.3, which would slash domestic diesel fuel consumption of 10 billion gallons per year by 25-30%.

A 50% reduction in drag would require very aggressive (and costly) reengineering. Yet the U.S. Department of Energy's Office of FreedomCAR and Vehicle Technologies, which funds Argonne's research as part of a seven-member aerodynamic drag reduction consortium, believes it can cost-effectively reduce drag by 20%. Even trimming tractor-trailer drag by a mere 6% could slash fuel costs $1.5 billion or more annually, says Dave Pointer.

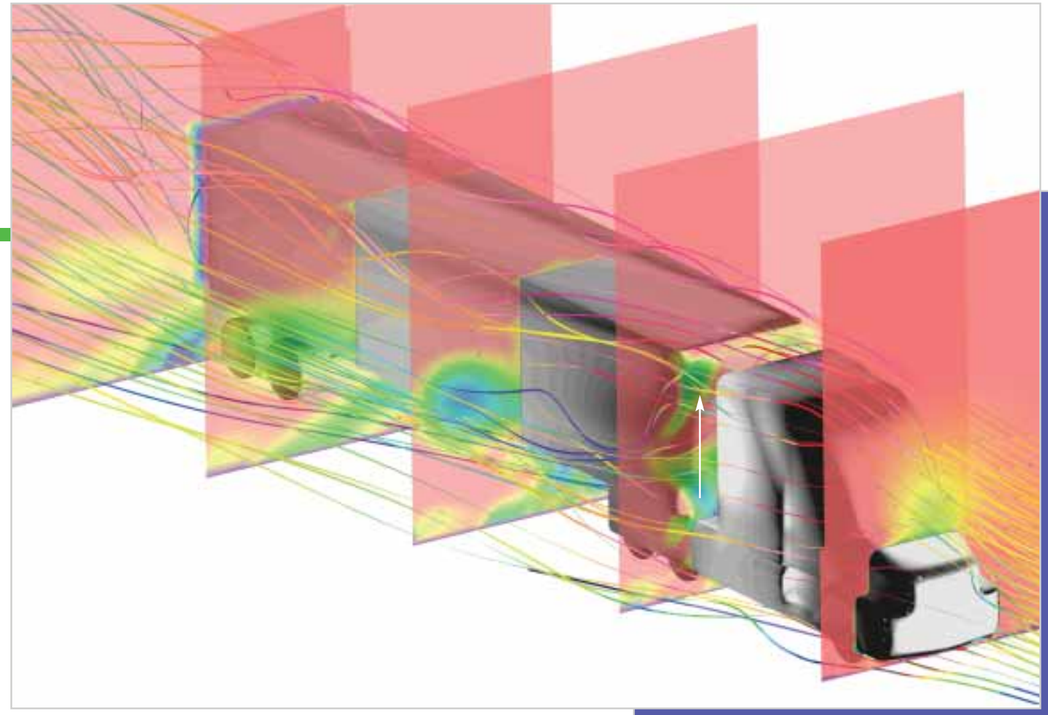
To reach that modest goal, truck makers must overcome substantial inertia. Drivers like the in-your-face, non-aerodynamic styling of their big rigs. Fleet owners claim good drivers do more to stretch fuel economy than could any redesign.

Most importantly, truck makers have limited analytical capabilities to assess aerodynamic design, says Weber. Until now, they have mostly used wind tunnels to test truck designs for drag. That involves crafting costly models, renting expensive wind tunnels, outfitting them with sensors for testing — and then redoing the entire process for each design modification. This trial-and-error process not only is slow and expensive, but often fails to show how tractors interact with their trailers.

Fluid

A mathematical technique called computational fluid dynamics (CFD) promises to change this. It models the stresses created by the flow of air around an object. This is done by breaking the surface of the object into small chunks, or cells, and calculating each cell's interaction with the flow of air as it is perturbed by other cells. It takes about 1 to 6 million cells to build a simplified tractor-trailer model, Pointer estimates. Realistic truck geometries would require 12–15 million cells.

Even trimming tractor-trailer drag by a mere 6% could slash fuel costs by $1.5 billion or more annually.



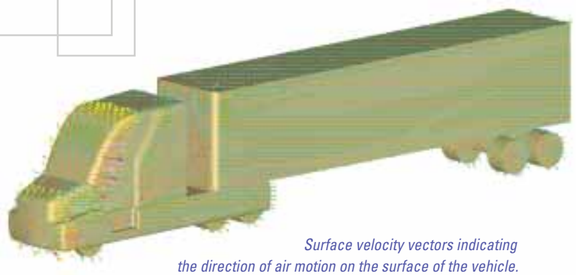
Streamlines showing predicted motion of air over the vehicle at a yaw angle of 10 degrees (equivalent to a truck traveling at 70 miles per hour with a crosswind of approximately 12 miles per hour). Streamline color and translucent contour planes indicate local velocity magnitude. Surface shading indicates surface pressure coefficient distribution.

Crunching those numbers requires a supercomputer. Automakers have being doing these types of calculations since the 1980s, relying on costly supercomputers. Because they produced millions of cars annually, they could afford the expense. Truck manufacturers, who build fewer Class 8 trucks in a year than the auto industry churns out vehicles in a week, could not.

Things began to change in 1994. That was when researchers turned on the first Beowulf cluster, a high-performance network of cheap, off-the-shelf PCs designed to break complex operations down into chunks and process them in parallel. Beowulf clusters achieve supercomputer performance at a price that moderate sized businesses can afford. They are especially well suited for CFD because models determine forces by running parallel calculations on millions of cells.

The problem, says Weber, lies in applying supercomputing power to tractor-trailers. Most tractor-trailer companies are likely to operate small Beowulf clusters. CFD would make heavy demands on their number crunching capabilities. If manufacturers had to run large CFD models on small clusters, they would find it painfully slow to find the right combination of cell size, quantity, and distribution to speed calculations without surrendering accuracy.

The mission of Weber's team is to use Argonne's large 80- and 350-PC Beowulf clusters to rapidly ascertain the best modeling practices for tractor-trailer CFD models. This



Surface velocity vectors indicating the direction of air motion on the surface of the vehicle. Vector color indicates velocity magnitude — full body view

COLLABORATORS

W. David Pointer (B.S., M.S., Ph.D., Nuclear Engineering, University of Tennessee) is a member of the research staff of the Nuclear Engineering Division of Argonne National Laboratory. Dr. Pointer's experience in the field of fluid dynamics and heat transfer allows him to pursue a wide variety of research areas, but his primary interest is in the identification, analysis, and control of fluid dynamic instabilities. Dr. Pointer is currently applying advanced computational and experimental fluid dynamics methods to the design and development of a wide range of systems such as class 8 tractor-trailer vehicles, advanced high-temperature gas-cooled nuclear power plants and high-power-density liquid-metal-cooled accelerator target systems.

David Weber received his Ph.D. from the University of Illinois, Champaign-Urbana, Illinois, in 1974 in Nuclear Engineering. He has over 30 years experience in computational science and engineering, computational fluid dynamics, high performance computing and nuclear reactor safety. Dr. Weber is currently the director of new program development for engineering research at ANL.

Tanju Sofu received his Ph.D. in Nuclear Engineering from the University of Tennessee, Knoxville, Tennessee in 1992. Dr. Sofu is currently the Engineering Simulation Section Manager in the Nuclear Engineering Division. He is responsible for coordinating various nuclear and non-nuclear engineering simulation projects, particularly those involving computational fluid dynamics support for advanced reactor designs and transportation-related initiatives.

Further Reading:

Pointer, W. David *Evaluation of Commercial CFD Code Capabilities for Prediction of Heavy Vehicle Drag Coefficients*, Proceedings of the 2004 AIAA Fluid Dynamics Conference and Exhibition, Portland, OR, June 2004, AIAA-2004-2254.

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involves testing modeling strategies and then validating the results against detailed data from wind tunnel tests. The resulting guidelines will give truck designers the confidence to use CFD to replace more expensive trial-and-error testing.

Building a Model

To build a CFD model, Weber's team starts with the Generic Conventional Model (GCM), a simplified, one-eighth-scale representation of a Class 8 truck used for wind tunnel research at NASA Ames Research Center in California. At 7 feet 10 inches long by 2 feet 6 inches wide, it is somewhat larger than Shaquille O'Neal and decked out with 490 pressure sensors, with an additional 368 on the wind tunnel walls and floor.

Argonne's first step is to create a mathematical representation of the physical GCM model. DOE's team does this by making pinpoint optical measurements of the model. This creates a three-dimensional "cloud" that defines the surface of the vehicle. Computer-aided design (CAD) software then imports the cloud scan and converts it into a three-dimensional solid surface that consists of millions of triangles, each defining a flat surface.

"The resulting surface definition is not ideal," says Pointer. "Many of the surfaces are confusing or have small holes." In most models, 0.1 mm holes are inconsequential; in CFD models, they create wind eddies that play havoc with aerodynamic calculations.

Pointer cleans up the model by use of a process called wrapping. First, he creates a solid box the same size as the wind tunnel. It consists of three-dimensional cells, called bricks, whose lengths range from 0.5 mm to 16 mm. He then positions the tractor-trailer model in the center of the tunnel. The planes where the tractor-trailer surface passes through the bricks define the new surface. Since the bricks are larger in scale than the imperfections, they do not capture the flaws from the old surface.

The model is not yet precise enough to use. Pointer has to refine such critical features as axles, exhaust stacks, door handles, and rear view mirrors (which can account for up to 15% of all drag). He then cuts away the volume of the truck, leaving behind a cavity that looks like a mold used to make plastic trucks. Next, he blends the surrounding brick cells with a thin layer of three-dimensional polyhedral cells to better represent the wrapped surface. This reduces the number of cells in the model and the number of calculations required to solve CFD problems.

Two types of cells surround the detailed truck cutout. The first are called near-vehicle cells; they represent the space where air moves within a truck-width of the vehicle. The cells are smaller (and produce more precise calculations) around mirrors, axles, and other critical features. They grow larger further away from the truck, where precise calculation is less important.

The second type of cell is called near-wall. It represents flow close to the surface. "If we let the CFD system take its course, we would wind up with billions of small cells," says Tanju Sofu. "Finding the right cell size is an art, and how to determine it represents an important guideline to industry."

Turbulence

Once the researchers have specified the CFD model, they need to describe the flow of air around the truck. In a perfect aerodynamic body, explains Sofu, air would flow in an orderly fashion. Each airstream would move at its own speed and direction. Air molecules would not cross airstream boundaries or bump into each other. In real life, though, air molecules collide and change one another's motion all the time. This creates eddies that range in size from micrometers to tens of centimeters.

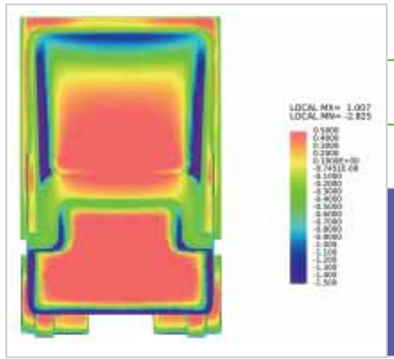
Modeling turbulence across different size scales is far from trivial. CFD software attacks the problem with Navier-Stokes equations, differential equations that describe the turbulent motion of the air space by taking into account conservation of mass, linear momentum, and energy. "Navier-Stokes is perfectly capable of representing the flow field," says Pointer. "But if you use it to try to solve the smallest scale eddies, you end up with a model with trillions of cells that is impossible to resolve with the most powerful computers today."

"That's why you need a turbulence model," adds Sofu. "Instead of trying to resolve each small-scale eddy, the model represents their influence as a statistical fluctuation about some average value of velocity."

Turbulence models differ from one another in how they view the relationship between stress and strain in flow fields caused by small eddies, Sofu continues. One method presumes a linear relationship, so doubling stress doubles strain. High-order turbulence models use cubic or quadratic functions that increase strain exponentially for every step-up in stress. Other high-order models introduce additional equations to relate stress to strain increase, adding to the computational burden of the model.

Moving Forward

Just as they did when optimizing cell size and distribution, the Argonne team seeks to achieve the most accurate turbulence model using the least amount of computing power. The only way to determine the parameters of this sweet spot is to test the CFD model against wind tunnel data.



Predicted pressure coefficients on the surface of the GCM — front view.

Looking at drag alone is not sufficient to validate a model. Instead, Weber, Pointer, and Sofu examine velocity, viscosity, and vorticity. Velocity describes cell-to-cell changes in air speed and direction. Viscosity measures how well the model incorporates eddies; a good turbulence model reflects how eddies slow and mix the airstream to make it more viscous. Finally, they measure vorticity, the tendency of a flow to rotate about an axis.

The reason the wind tunnel model carries 490 pressure sensors is to provide the detailed data needed to truly validate the CFD model. This ensures that the simulation fully captures the aerodynamic complexities of a moving truck. That way, truck manufacturers will have confidence in translating Argonne's results into models of their own.

Still, Argonne's research remains a work in progress. Pointer and Sofu continue to do parametric studies to optimize cell size and turbulence models. They have already proven their models are 99% accurate. More importantly for manufacturers with smaller supercomputers, the best practices they have pioneered can achieve 95% accuracy at speeds fast enough for practical business use on small Beowulf clusters.

That's good enough to promise real aerodynamic improvements in the near future. So while Class 8 trucks are likely to remain the dreadnoughts of the highway, they promise to be more fuel efficient and economical than ever before.

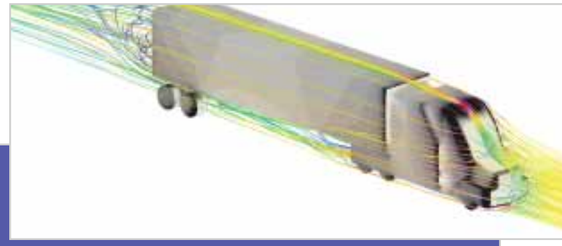
FROM NUCLEAR POWER TO TRUCK AERODYNAMICS

>> ***Automotive research was far from Dave Weber's mind when researchers from General Motors Corp. visited Argonne National Laboratory 10 years ago. The GM team came to Argonne to learn how Weber used supercomputers to model thermohydraulics, fluid dynamics, and structural dynamics to ensure the safety of nuclear reactors.***

"They didn't find the nuclear part interesting, but the fluid dynamics was similar to work they did on aerodynamics, combustion, and internal automotive fluid flows," Weber recalls. The interest soon blossomed into Argonne's membership in the Supercomputer Automotive Applications Partnership, which brought together automotive researchers and five Department of Energy (DOE) laboratories.

"They wanted a partner in the development of next generation software for fluid dynamics analysis," Weber relates. "CD adapco, a commercial CFD software company, was selected for possible commercialization of this software, which would complement their product STAR-CD," says Weber. "We developed a good working relationship with the vendor and were favorably impressed with the Star-CD code. "

Later, when DOE began working with truck manufacturers to address aerodynamic drag, engineers were skeptical that commercially available CFD codes could adequately represent vehicles. "We were already familiar with STAR-CD and we could independently verify it," says Weber. "While other consortium members are focusing on long-term research, we are addressing near-term needs so truck manufacturers can begin using CFD now."



Streamlines showing predicted motion of air over the vehicle. Streamline color indicates local velocity magnitude. Surface shading indicates surface pressure coefficient distribution.

Laura Painton Swiler

Laura Painton Swiler's MISSION IS TO USE COMPUTATIONAL MODELS to help others predict the future and make better decisions. But it was New Jersey's infamous homeless garbage barge that helped determine her future.

The environmental fiasco of a homeless garbage barge helped convince Swiler to leave a well-paid job at Bell Labs in 1991 and pursue a Ph.D. in Engineering and Public Policy at Carnegie Mellon University. "I was in a very idealistic phase of life and wanted to use my capabilities to improve our world," says the DOE CSGF alumna, whose dissertation dealt with models of optimization under uncertainty.

For the past decade, Swiler has been applying her vision and scientific prowess to a wide range of prognostics, system reliability and optimization projects of national importance as a Technical Staff member at DOE's Sandia National Laboratories in Albuquerque, New Mexico.

> "You never know where your research is going to end up."

Her first project at Sandia was to help develop an algorithm to balance false negative and positive readings from onboard emissions diagnostic sensors, mandated by the EPA in 1996 and now part of the emission-light feature in all new cars.

She has also provided decision analysis support for DOE's Waste Isolation Pilot Plant (WIPP) and Rocky Flats nuclear waste repository siting and disposal projects. Most recently, Swiler led a research project, in collaboration with Lockheed Martin, to develop prognostic algorithms for the F-16 accessory drive gearbox in order to allow for less-expensive predictive, rather than routine, maintenance.

Her long-term research baby emerged in 1997 as a DARPA-funded project to apply risk assessment techniques to cybersecurity. For four years, Swiler and Sandia colleague Cindy Phillips worked to develop highly detailed attack graphs. These mapped attack possibilities against specific network configurations and topologies.

Disappointingly, however, project funding ended before the "combinatorial explosion" of the graphs was solved, seemingly signaling the work's demise.

Then earlier this year, Swiler was visited by staff from Skybox, a small high-tech start-up, who hailed her and Phillips as "the mothers of the attack graph."

Based on a simplified version of the attack graph work, Skybox has produced a successful, easy-to-use commercial cybersecurity tool.

"When I learned this, I felt very gratified. I thought, 'Hey, someone has taken our idea, they're supporting several dozen people at a small company and they're helping companies make their networks more secure,'" says Swiler. "You never know where your research is going to end up."

Or you yourself. After nine years of working on highly applied "work for others" projects as part of Sandia's Systems Reliability Group, Swiler moved last year to the Lab's Optimization and Uncertainty Estimation Department.

Here she's back to thinking about modeling uncertainty, specifically as it relates to calibrating parameters of large computer codes.

"It's interesting even within Sandia how different the atmosphere can be," says Swiler, who's now juggling boning-up on the latest uncertainty research with the everyday uncertainties of being a mother of a three-year-old and a five-year-old. "In my old group, no one published much. In this group, one's performance is assessed by publications. It's much more of an academic environment."

Paul Bunch

THE JOURNEY FROM THE LAB to senior corporate management has taught Paul Bunch one key thing about mathematical models of business optimization: They're only human.

"When you start in business after graduate school, you tend to think that the model gives you the answer, a magic bullet," says Bunch, a Senior Manager, Capacity Planning and Project Management, with pharmaceutical giant Eli Lilly and Company.

"But what you realize is that when you're trying to incorporate modeling into a large business, the models don't give you the answer you're actually going to implement, but rather a large number of options that aid in executives' decision-making processes."

Nonetheless, Bunch says that in his seven years with the company, modeling has become increasingly important in the decision-making process.

The Purdue University graduate's first modeling projects at Indianapolis-based Eli Lilly involved maximizing the efficiency of plant scheduling and facility design. Now, his six-person group's models involve R&D capacity management across the Eli Lilly empire. These optimization models include everything from R&D inputs and processes to human resources, costs and financial risk-benefit calculations covering as many as 100 concurrent drug development projects.

"We spend more than $2 billion a year, or about $9 million a work day, on R&D," notes Bunch of a company with about 46,000 employees, approximately 8,700 of whom are doing R&D. "So you say, 'Gosh, it's worthwhile to devote some people to optimization modeling.'"

Indeed, says Bunch, optimization modeling and simulation methodologies have become an industry standard, a fact driven in part by increased competition and therefore internal pressure for greater efficiency. This growth in modeling has also been fuelled by improvements in optimization software, which is now increasingly user-friendly.

"When we started using these tools in the late 1990s, we were typing in code to describe problems," says Bunch, who is one of a new generation of computational scientists rising through the ranks of corporate management.

The increased speed offered by optimization tools has also made them part of everyday planning.

"Where optimization becomes relevant is when you can get an answer in a time within which it can be used to affect a decision, and this is often hours or days," says Bunch.

As a case in point, the algorithms he developed for his thesis on the perfect B-matching problem, which at the time he admits "seemed quite irrelevant", are now part of commonly used commercial optimization software.

While increasingly sophisticated models are key to providing accurate advice, Bunch, who's the boardroom face of Eli Lilly's modeling group, says it's still crucial to communicate these results to senior executives for whom mention of algorithms is fog in front of the bottom line.

Says Bunch: "If you don't get to the point where you realize you have to adjust the information that you share, you really won't be effective."

> …optimization modeling and simulation methodologies have become an industry standard…

Martin Bazant

AS A NEWLY APPOINTED PROFESSOR of applied mathematics at the Massachusetts Institute of Technology (MIT) in 2000, Martin Bazant knew that attracting a research group was a key challenge. An emeritus professor offered this advice: Build a unique graduate course and they will come. And they have.

Bazant's course, Random Walks and Diffusion, has become his academic shingle, defining his creative, independent, and mixed applied-theoretical approach to research — one that is dramatically changing our understanding of granular movement.

"If you didn't know which department I was in and looked at all my research projects, you'd have a hard time classifying me," says Bazant, now an Associate Professor in MIT's Mathematics Department.

Bazant thrives at the intersection of computational science, physics (his Ph.D. discipline), applied mathematics and engineering. His work includes experimental projects, computational modeling and theory.

> "If you didn't know which department I was in and looked at all my research projects, you'd have a hard time classifying me."

He's working to integrate the understanding of the individual random walks of particles with their group behavior in a dense granular flow, such as sand in an egg-timer.

"We don't have a microscopic understanding of what's happening in dense granular flow," says Bazant, whose vibrant lab is staffed with an eclectic mix of five graduate students, mostly recruited from his signature course. "My goal is to generalize the concept of the random walk for strongly interacting systems, such as granular and glassy materials, dominated by packing constraints."

In experiments in his Dry Fluids Lab, Bazant has already significantly redefined our understanding of granular flow. The lab contains a massive gumball machine-like device which holds 100,000 small pellets whose descending motion is recorded by a high-speed video camera.

The only prior microscopic model for granular drainage is based on the concept of voids, or missing particles, undergoing independent random walks upward from the outlet.

"We've found that the void model is totally wrong," says Bazant, who received a 2002 Department of Energy (DOE) Early Career PI award. "Instead, a particle moves cooperatively in 'spots', largely preserving its cage of nearest neighbors."

His group is performing large-scale simulations of granular flow in collaboration with researchers at DOE's Sandia National Laboratory. They're also running simulations on the lab's 32-processor Beowulf cluster using Bazant's Spot Model, a new mathematical theory of cooperative diffusion.

The work has important applications to the modeling and design of new pebble-bed nuclear reactors. Bazant has a patent pending on a guide ring designed for MIT's prototype pebble-bed reactor that optimizes the composition and mixing of radioactive and moderating 'pebbles', a critical factor for safe and efficient reactor function.

Bazant's group is also applying its understanding of microscopic movement to a new approach — which uses AC electric fields — to pumping and mixing in microfluidic devices. Their prototype device could greatly accelerate some biological assays by using fluid flow to speed the random walks of probe molecules.

After five years of intense research, and now with dreams of writing a book on random walks and diffusion, Bazant is up for tenure next year. If family tradition counts for anything, his chances of receiving it are at anything but random odds: He's the fourth consecutive generation science professor in the Bazant lineage.

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 Science 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.

One of Howes' responsibilities was to oversee the Department of Energy's Computational Science Graduate Fellowship (DOE CSGF) program. He was extremely committed to this program. In fact, without his support, the program may not have survived.

To honor his memory and his dedication to the DOE CSGF program, one or two DOE CSGF fellows are chosen each calendar year as a Howes Scholar. Candidates are chosen on the basis of their academic excellence, leadership and character and are nominated by their academic advisors. The honor provides the recipients with a substantial cash award, a Tiffany crystal paperweight, and the distinction of being named a Howes Scholar.

2004 Scholar

Collin Wick, a DOE CSGF fellow from 2000-2003, was selected as the 2004 Howes Scholar. Graduating from the University of Minnesota with a Ph.D. in Computational Chemistry, Dr. Wick spent time at the National Technical University in Athens, Greece, before returning to the United States in July to take a position with Pacific Northwest National Laboratory in Richland, Washington.

Dr. Wick attended the 2004 annual DOE CSGF fellows conference held in Washington DC, where he presented his research and accepted his award. Dr. Margaret Wright of the Courant Institute presented the award, and Mary Hall, Dr. Howes' widow, was in attendance.

Special Presentation

Because Dr. Jon Wilkening, a 2003 Howes Scholar recipient, was unable to attend the 2003 awards ceremony, he was invited to present his research and to be recognized at the 2004 ceremony luncheon. Dr. Wilkening presented his research and was recognized as a Howes Scholar.

For More Information

Contact Barbara Helland at helland@krellinst.org for more information regarding this award.

Margaret Wright, Mary Hall, Jon Wilkening, Collin Wick, Barbara Helland and David Brown at the awards ceremony during the annual DOE CSGF fellows conference.

Collin Wick presents his research at the annual DOE CSGF fellows conference.

Jon Wilkening fields questions from current fellows as he discusses his research at the annual DOE CSGF fellows conference.

Alumni Directory

A
B
C

A

Asohan Amarasingham
Brown University
Cognitive Science
Fellowship Years: 1998-2002
Current Status: Staff, University of Jaffna, Sri Lanka

Matthew Anderson
University of Texas
Physics
Fellowship Years: 2000-2004
Current Status: Staff, Louisiana State University

B

Allison Baker
University of Colorado
Applied Mathematics
Fellowship Years: 1999-2003
Current Status: Lawrence Livermore National Laboratory

Devin Balkcom
Carnegie Mellon University
Robotics
Fellowship Years: 2000-2004
Current Status: Faculty, Dartmouth College

Edward Barragy
University of Texas
Engineering Mechanics
Fellowship Years: 1991-1993
Current Status: Intel

William Barry
Carnegie Mellon University
Structural & Computational Engineering
Fellowship Years: 1994-1998
Current Status: Faculty, Asian Institute of Technology

Martin Bazant
Harvard University
Physics
Fellowship Years: 1992-1996
Current Status: Faculty, Massachusetts Institute of Technology

Bonnie Carpenter Beyer
University of Illinois
Mechanical Engineering
Fellowship Years: 1991-1995
Current Status: Rockwell Collins

Edwin Blosch
University of Florida
Aerospace Engineering
Fellowship Years: 1991-1994
Current Status: CFD Research Corp

Dean Brederson
University of Utah
Computer Science
Fellowship Years: 1996-1998
Current Status: Staff, University of Utah

Paul Bunch
Purdue University
Chemical Engineering
Fellowship Years: 1994-1997
Current Status: Eli Lilly & Company

Jeffery Butera
North Carolina State University
Mathematics
Fellowship Years: 1993-1997
Current Status: Staff, Hampshire College

C

Brandoch Calef
University of California – Berkeley
Applied Mathematics
Fellowship Years: 1996-2000
Current Status: Boeing

Patrick Canupp
Stanford University
Aerospace Engineering
Fellowship Years: 1991-1995
Current Status: Joe Gibbs Racing

Kent Carlson
Florida State University
Mechanical Engineering
Fellowship Years: 1991-1995
Current Status: Staff, University of Iowa

Nathan Carstens
Massachusetts Institute of Technology
Nuclear Engineering
Fellowship Years: 2001-2004
Current Status: Student, MIT

Edward Chao
Princeton University
Plasma Physics
Fellowship Years: 1992-1995
Current Status: GE Medical Systems

Jarrod Chapman
University of California – Berkeley
Computational Biology
Fellowship Years: 1999-2003
Current Status: Student, University of California – Berkeley

Eric Charlton
University of Michigan
Aerospace Engineering
Fellowship Years: 1992-1996
Current Status: Lockheed Martin

Michael Chiu
Massachusetts Institute of Technology
Mechanical Engineering
Fellowship Years: 1992-1996
Current Status: Teradyne

Joshua Coe
University of Illinois
Chemical Physics
Fellowship Years: 2001-2002
Current Status: Student, University of Illinois

Gavin Conant
University of New Mexico
Biology
Fellowship Years: 2000-2004
Current Status: Staff, Universitat Leipzig in Germany

Ken Comer
North Carolina State University
Mechanical Engineering
Fellowship Years: 1991-1995
Current Status: Procter & Gamble

John Costello
University of Arizona
Applied Mathematics
Fellowship Years: 1998-2002
Current Status: Student, University of Arizona

Nathan Crane
University of Illinois
Civil Engineering
Fellowship Years: 1999-2002
Current Status: Sandia National Laboratories — New Mexico

Stephen Cronen-Townsend
Cornell University
Computational Materials Physics
Fellowship Years: 1991-1995
Current Status: Staff, University of Massachusetts

Robert Cruise
Indiana University
Physics
Fellowship Years: 1997-2001

Joseph Czyzyk
Northwestern University
Industrial Engineering
Fellowship Years: 1991-1994

D

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

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

John Dolbow
Northwestern University
Theoretical and Applied Mechanics
Fellowship Years: 1997-1999
Current Status: Faculty, Duke University

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

Amanda W. Duncan
University of Illinois
Electrical Engineering
Fellowship Years: 1991-1995
Current Status: Intel

Lewis Jonathan Dursi
University of Chicago
Astrophysics
Fellowship Years: 1999-2003
Current Status: Canadian Institute for Theoretical Astrophysics

E

Ryan Elliott
University of Michigan
Aerospace Engineering
Fellowship Years: 2000-2004
Current Status: Staff, University of Michigan

Thomas Epperly
University of Wisconsin – Madison
Chemical Engineering
Fellowship Years: 1991-1995
Current Status: Lawrence Livermore National Laboratory

F

Matthew Fago
California Institute of Technology
Aeronautical Engineering
Fellowship Years: 2000-2003
Current Status: Northrop Grumman Space Technology

Michael Falk
University of California – Santa Barbara
Physics
Fellowship Years: 1995-1998
Current Status: Faculty, University of Michigan

Matthew Farthing
University of North Carolina
Environmental Science & Engineering
Fellowship Years: 1997-2001
Current Status: Staff, University of North Carolina

Michael Feldmann
California Institute of Technology
Computational Chemistry
Fellowship Years: 1999-2002
Current Status: Network Computing Services, Inc.

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

Robert Fischer
Harvard University
Computer Science
Fellowship Years: 1994-1998
Current Status: Brigham and Women's Hospital

Gregory Ford
University of Illinois
Chemical Engineering
Fellowship Years: 1993-1995

Oliver Fringer
Stanford University
Environmental Fluid Mechanics
Fellowship Years: 1997-2001
Current Status: Faculty, Stanford University

G

Kenneth Gage
University of Pittsburgh
Chemical Engineering
Fellowship Years: 1998-2002
Current Status: Student, University of Pittsburgh

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

Charles Gerlach
Northwestern University
Mechanical Engineering
Fellowship Years: 1995-1999
Current Status: Network Computing Services, Inc.

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

Christopher Gesh
Texas A&M University
Nuclear Engineering
Fellowship Years: 1993-1997
Current Status: Pacific Northwest National Laboratory

Matthew Giamporcaro
Boston University
Cognitive and Neural Systems
Fellowship Years: 1998-2000
Current Status: Adaptive Optics Associates

Kevin Glass
University of Oregon
Computer Science
Fellowship Years: 1996-2000
Current Status: Staff, University of Oregon

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

D
E
F
G

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

Catherine Grasso
Cornell University
Bioinformatics
Fellowship Years: 2000-2004
Current Status: Staff, University of Michigan

Corey Graves
North Carolina State University
Computer Engineering
Fellowship Years: 1996-1999
Current Status: Faculty, North Carolina Agricultural & Technical State University

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

Boyce Griffith
New York University – Courant Institute
Applied Mathematics
Fellowship Years: 2000-2004
Current Status: Student, New York University

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

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

H

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

Glenn Hammond
University of Illinois
Environmental Engineering & Science
Fellowship Years: 1999-2003
Current Status: Sandia National Laboratories – New Mexico

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

Rellen Hardtke
University of Wisconsin – Madison
Physics
Fellowship Years: 1998-2002
Current Status: Faculty, California Polytechnic State University

Eric Held
University of Wisconsin – Madison
Engineering Physics
Fellowship Years: 1995-1999
Current Status: Faculty, Utah State University

Judith Hill
Carnegie Mellon University
Mechanics, Algorithms & Computing
Fellowship Years: 1999-2003
Current Status: Faculty, Carnegie Mellon University

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

Jeffrey Hittinger
University of Michigan
Aerospace Engineering & Scientific Computing
Fellowship Years: 1996-2000
Current Status: Lawrence Livermore National Laboratory

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

Daniel Horner
University of California – Berkeley
Chemistry
Fellowship Years: 2000-2004
Current Status: Lawrence Berkeley National Laboratory

William Humphrey
University of Illinois
Physics
Fellowship Years: 1992-1994
Current Status: TurboLabs, Inc.

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

E. McKay Hyde
California Institute of Technology
Applied & Computational Mathematics
Fellowship Years: 1999-2002
Current Status: Faculty, Rice University

I

Eugene Ingerman
University of California – Berkeley
Applied Mathematics
Fellowship Years: 1997-2001
Current Status: Staff, University of California – Davis

Ahmed Ismail
Massachusetts Institute of Technology
Chemical Engineering
Fellowship Years: 2000-2004
Current Status: Student, Massachusetts Institute of Technology

J

Nickolas Jovanovic
Yale University
Mechanical Engineering
Fellowship Years: 1992-1994
Current Status: Faculty, University of Arkansas – Little Rock

K

Benjamin Keen
University of Michigan
Mathematics
Fellowship Years: 2000-2004
Current Status: IDA Center for Computing Sciences

Jeremy Kepner
Princeton University
Computational Cosmology
Fellowship Years: 1993-1996
Current Status: Staff, Massachusetts Institute of Technology

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

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

Justin Koo
University of Michigan
Aerospace Engineering
Fellowship Years: 2000-2004
Current Status: Student, University of Michigan

Michael Kowalok
University of Wisconsin
Medical Physics
Fellowship Years: 2000-2004
Current Status: Student, University of Wisconsin

Yury Krongauz
Northwestern University
Theoretical & Applied Mechanics
Fellowship Years: 1993-1996

L

Eric Lee
Rutgers University
Mechanical Engineering
Fellowship Years: 1999-2003
Current Status: Staff, Northeastern University

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

Lars Liden
Boston University
Cognitive & Neural Systems
Fellowship Years: 1994-1998
Current Status: Staff, University of Washington

Tasha (Palmer) Lopez
University of California – Los Angeles
Chemical Engineering
Fellowship Years: 2000-2001
Current Status: IBM

Christie Lundy
University of Missouri – Rolla
Physics
Fellowship Years: 1991-1994
Current Status: State of Missouri Employee

M

William Marganski
Boston University
Biomedical Engineering
Fellowship Status: 1998-2002
Current Status: Boston Biomedical Research Institute

Daniel Martin
University of California – Berkeley
Mechanical Engineering
Fellowship Years: 1993-1996
Current Status: Lawrence Berkeley National Laboratory

Marcus Martin
University of Minnesota
Physical Chemistry
Fellowship Years: 1997-1999
Current Status: Sandia National Laboratories – New Mexico

Richard McLaughlin
Princeton University
Applied Mathematics
Fellowship Years: 1991-1994
Current Status: Faculty, University of North Carolina

Lisa Mesaros
University of Michigan
Aerospace Engineering & Scientific Computing
Fellowship Years: 1991-1995
Current Status: FLUENT, Inc.

Richard Mills
College of William and Mary
Computer Science
Fellowship Years: 2001-2004
Current Status: Oak Ridge National Laboratory

Erik Monsen
Stanford University
Aerospace and Astronautical Engineering
Fellowship Years: 1991-1994
Current Status: Student, University of Colorado

Brian Moore
North Carolina State University
Nuclear Engineering
Fellowship Years: 1992-1995
Current Status: Global Nuclear Fuel

James (Dan) Morrow
Carnegie Mellon University
Robotics
Fellowship Years: 1992-1995
Current Status: Sandia National Laboratories – New Mexico

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

N

Heather Netzloff
Iowa State University
Physical Chemistry
Fellowship Years: 2000-2004
Current Status: Staff, Iowa State University

Pauline Ng
University of Washington
Bioengineering
Fellowship Years: 2000-2002
Current Status: Illumina

Brian Nguyen Gunney
University of Michigan
Aerospace Engineering & Scientific Computing
Fellowship Years: 1993-1996
Current Status: Lawrence Livermore National Laboratory

Diem-Phuong Nguyen
University of Utah
Chemical Engineering
Fellowship Years: 1999-2003
Current Status: Staff, University of Utah

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

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

Catherine Norman
Northwestern University
Applied Mathematics
Fellowship Years: 2000-2004
Current Status: Student, Northwestern University

O

Christopher Oehmen
University of Memphis
Biomedical Engineering
Fellowship Years: 1999-2003
Current Status: Pacific Northwest National Laboratory

P

Steven Parker
University of Utah
Computer Science
Fellowship Years: 1994-1997
Current Status: Faculty, University of Utah

Joel Parriott
University of Michigan
Astronomy & Astrophysics
Fellowship Years: 1992-1996
Current Status: Office of Management and Budget

Virginia Pasour
North Carolina State University
Biomathematics
Fellowship Years: 1998-1999
Current Status: Student, Cornell University

Robert (Chris) Penland
Duke University
Biomedical Engineering
Fellowship Years: 1993-1997
Current Status: Predix Pharmaceuticals, Inc.

James Phillips
University of Illinois
Physics
Fellowship Years: 1995-1999
Current Status: Staff, University of Illinois

Todd Postma
University of California – Berkeley
Nuclear Engineering
Fellowship Years: 1994-1998
Current Status: Totality

Richard Propp
University of California – Berkeley
Mechanical Engineering
Fellowship Years: 1993-1996
Current Status: Real Time Solutions

Q

Alejandro Quezada
University of California – Berkeley
Geophysics
Fellowship Years: 1997-1998

R

Nathan Rau
University of Illinois
Civil Engineering
Fellowship Years: 2000-2001
Current Status: Hanson Professional Services

Clifton Richardson
Cornell University
Physics
Fellowship Years: 1991-1995

John Rittner
Northwestern University
Mechanical Engineering
Fellowship Years: 1991-1995
Current Status: Chicago Board Options Exchange

Courtney Roby
University of Colorado
Electrical Engineering
Fellowship Years: 2002-2003
Current Status: Student, University of Colorado

David Ropp
University of Arizona
Applied Mathematics
Fellowship Years: 1992-1995
Current Status: Sandia National Laboratories – New Mexico

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

S

Robert Sedgewick
University of California – Santa Barbara
Physics
Fellowship Years: 2000-2003
Current Status: Staff, University of Pittsburgh

Susanne (Essig) Seefried
Massachusetts Institute of Technology
Aeronautics/Astronautics
Fellowship Years: 1997-2002

Marc Serre
University of North Carolina
Environmental Science & Engineering
Fellowship Years: 1996-1999
Current Status: Faculty, University of North Carolina

Elsie Simpson Pierce
University of Illinois
Nuclear Engineering
Fellowship Years: 1991-1993
Current Status: Lawrence Livermore National Laboratory

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

Steven Smith
North Carolina State University
Chemical Engineering
Fellowship Years: 1992-1994
Current Status: E.I. DuPont

Eric Sorin
Stanford University
Chemical Physics
Fellowship Years: 2002-2004
Current: Student, Stanford University

Scott Stanley
University of California – San Diego
Mechanical Engineering
Fellowship Years: 1994-1998
Current Status: Hewlett Packard Company

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

Rajeev Surati
Massachusetts Institute of Technology
Electrical Engineering & Computer Science
Fellowship Years: 1995-1997
Current Status: Nexaweb

Laura (Painton) Swiler
Carnegie Mellon University
Engineering & Public Policy
Fellowship Years: 1992-1995
Current Status: Sandia National Laboratories – New Mexico

T

Shilpa Talwar
Stanford University
Scientific Computing
Fellowship Years: 1992-1994
Current Status: Sandia National Laboratories – California

Mayya Tokman
California Institute of Technology
Applied Mathematics
Fellowship Years: 1996-2000
Current Status: Faculty, University of California – Berkeley

Mario Trujillo
University of Illinois
Mechanical Engineering
Fellowship Years: 1997-2000
Current Status: Staff, Pennsylvania State University

V

Anton Van Der Ven
Massachusetts Institute of Technology
Materials Science
Fellowship Years: 1996-2000
Current Status: Staff, Massachusetts Institute of Technology

Laura Vann Dominik
Florida Atlantic University
Electrical Engineering
Fellowship Years: 1993-1997
Current Status: Pratt & Whitney

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

Stephen Vinay
Carnegie Mellon University
Chemical Engineering
Fellowship Years: 1998-2000
Current Status: Bettis Laboratory

W

Phillip Weeber
University of North Carolina
Environmental Science & Engineering
Fellowship Years: 1994-1996
Current Status: Chatham Financial

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

Gregory Whiffen
Cornell University
Environmental Systems Engineering
Fellowship Years: 1991-1995
Current Status: NASA - Jet Propulsion Laboratory

Collin Wick
University of Minnesota
Computational Chemistry
Fellowship Years: 2000-2003
Current Status: Pacific Northwest National Laboratory

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

Jon Wilkening
University of California – Berkeley
Applied Mathematics
Fellowship Years: 1997-2001
Current Status: Staff, Courant Institute

Glenn Williams
University of North Carolina
Environmental Science & Engineering
Fellowship Years: 1993-1996
Current Status: Faculty, Old Dominion University

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

Lee Worden
Princeton University
Applied Mathematics
Fellowship Years: 1998-2002
Current Status: Staff, University of California – Davis

Peter Wyckoff
Massachusetts Institute of Technology
Chemical Engineering
Fellowship Years: 1992-1995
Current Status: Ohio Supercomputing Center

Z

Charles Zeeb
Colorado State University
Mechanical Engineering
Fellowship Years: 1993-1997
Current Status: Los Alamos National Laboratory

Scott Zoldi
Duke University
Theoretical & Computational Physics
Fellowship Years: 1996-1998
Current Status: Fair Issac Corporation

Marcelo Alvarez
University of Texas
Computational Astrophysics

Advisor:
Paul Shapiro
Practicum:
Los Alamos National Laboratory
Contact:
marcelo@astro.as.utexas.edu
Research Synopsis:
I am studying the formation of galaxies and large scale structure in the universe by numerical simulation. The focus of my work is the so-called cosmic "Dark Ages", after the universe became cool enough to transition from an ionized plasma to a neutral gas (recombination; 400,000 years old) but before the first few generations of stars and quasars emitted radiation that reionized it, making it once again an ionized plasma (cosmological reionization; hundreds of millions of years old). There is much excitement in this area today because recent observations such as those from the Wilkinson Microwave Anisotropy Probe (WMAP) have yielded interesting puzzles that challenge commonly held assumptions about how and when the first stars and quasars formed and how they affected further structure formation.

Kristopher Andersen
University of California – Davis
Physics

Advisor:
Warren Pickett
Practicum:
Oak Ridge National Laboratory
Contact:
keandersen@ucdavis.edu
Research Synopsis:
In my thesis research, I apply the computational tools of materials science to semiconductor quantum dots doped with magnetic transition elements. This research is motivated by two factors. First, current industrial trends toward miniaturization have stimulated research in materials with nanometer length scales. The size-dependent properties of quantum dots and advances in their fabrication have made semiconductor quantum dots a promising subset of the many proposed nanostructures. Second, semiconductor quantum dots with net magnetic moments may lead to novel device applications in the fields of spin-polarized magneteoelectronics, so-called spintronics, and quantum computing. By using density functional theory, I will be able to study magnetically doped semiconductor quantum dots grown from II-IV, II-VI, and IV-IV compounds. In this way research will provide insight into the application of these important nanostructures.

Annette Evangelisti
University of New Mexico
Computational Molecular Biology

Advisor:
Andreas Wagner
Practicum:
Los Alamos National Laboratory
Contact:
amevang@unm.edu
Research Synopsis:
My field of interest is computational molecular biology, in particular, gene expression and gene regulatory networks. DNA microarray technology now allows gene expression to be measured for an entire genome under differing conditions. This high-throughput technology provides a view of gene activity that permits fundamental exploration of gene expression and its underlying network of gene regulation. The challenge of microarray data analysis lies in discovery that is both biologically meaningful and statistically sound.

Sommer Gentry
Massachusetts Institute of Technology
Optimization/Control Theory

Advisor:
Eric Feron
Practicum:
Sandia National Laboratories – New Mexico
Contact:
sommerg@mit.edu
Notable:
Winner of IEEE Systems, Man, and Cybernetics Conference 2003 Best Student Paper award.
Research Synopsis:
Swing dancing is an example of a two-agent decentralized coordination system which uses only sensed information and no transmitted information. The leader in a dance couple plans the dance sequence in response to a song. Using some visual cues, the trajectory of his own body and hand, and the force applied at the dancing couple's connection points, the leader communicates to the follower a sequence of moves, which are selected from a small shared vocabulary.

This amazingly capable mechanism for coordination suggests design principles for human-automaton and automaton-automaton mobile systems, from surgical assistant robots to rover teams. I will investigate coordination in the dance model and applications of dance-inspired coordination techniques to automated agent teams. Coordination here refers to the selection of complementary primitives when direct communication of the primitives' alphabet element is not allowed.

Ahna Girshick
University of California – Berkeley
Vision Science

Advisor:
Martin Banks
Practicum:
Lawrence Berkeley National Laboratory
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Research Synopsis:
The understanding of the brain is certainly one of the most challenging scientific problems facing us. In particular, the mechanisms of vision not only are critical for survival but also integrate the study of a wide variety of brain functions at different levels. Vision is a field which attracts and aids scientists in a range of areas, from neuroscience and psychology to computer science, mathematics and engineering.

Vision Science seeks to explain how we see and how we can enable machines to see. One underlying problem of particular interest to me is that of correctly constructing a 3D scene from a set of 2-D images, in the face of multiple mathematically-correct answers. The term 'three-dimensional visual perception' describes the perception of 3D shape and space. The topic is significant because the percept of 3D space is critical survival knowledge for both biological organisms and many types of robots. Recent efforts have been shifted away from simple laboratory scenarios towards 'dynamic environments' in which both the observer and scene are in motion. This adjustment presents a range of exciting and challenging problems which I hope to focus on in my doctoral research.

Kristen Grauman
Massachusetts Institute of Technology
Computer Science

Advisor:
Trevor Darrell
Practicum:
Lawrence Berkeley National Laboratory
Contact:
kgrauman@mit.edu
Notable:
Received the Boston University Computer Science department's annual award for the outstanding senior in the graduating class. Received the Albert McGuinn award from the Boston College, College of Arts and Sciences, in 2001. Awarded Emerson Music Scholarship from the MIT Music department to support private piano study.
Research Synopsis:
My research interests are in computer vision and human-computer interfaces. Computer vision is the field of study devoted to building machines that can "see" or "recognize" things. Major goals include developing algorithms for the automatic analysis of image sequences, object recognition, shape and physical property analysis, and determination of the motion of both rigid and deformable bodies. High-performance computation is particularly critical for real-time applications that employ computer vision. The design and development of extremely powerful and complex systems will be necessary to effectively utilize computer vision techniques in practical applications in the near future.

I am specifically interested in the current limitations of the interfaces between humans and computers, and I feel that research in computer vision and other counterparts within artificial intelligence will allow us to surmount such obstacles.

Heath Hanshaw

University of Michigan
Nuclear Engineering

Advisor:
Edward Larsen
Practicum:
Los Alamos National Laboratory
Contact:
heathhanshaw@usa.net
Notable:
Received a Navy Commendation Medal for accomplishments while serving as faculty of the US Naval Academy Physics Department. Awarded the American Nuclear Society Scholarship in 2001-2003.
Research Synopsis:
My field is radiation transport theory, the computational science of simulating radiation particles (neutrons, photons, electrons, etc.) and their interactions with matter. The Boltzmann transport equation, a PDE with both hyperbolic and parabolic qualities, depending on the material and temperature regime, describes transport of radiation through phase space. The forward problem is to calculate the radiation transmitted, reflected, generated, and scattered through a known medium. The medium may be a plasma, a nuclear reactor, a drum of uncharacterized waste, or a medical patient. In the inverse problem, instead of calculating the radiation transported through a known medium, the unknown radiation source and properties of the medium are estimated from externally detected radiation. Important applications of inverse transport are remote sensing, medical imaging and radiotherapy, industrial non-destructive testing, and physics experiments.

Richard Katz

Columbia University
Geodynamics

Advisor:
Marc Spiegelman
Practicum:
Argonne National Laboratory
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Research Synopsis:
The goal of my research program is to better understand the role of subduction zones as a link between three of the Earth's chemically distinct planetary reservoirs: the hydrosphere, the crust and the mantle. Long-term evolution of these reservoirs depends critically on the flux of volatiles, sediments, and oceanic lithosphere through the 'fractionation machine' that is subduction. Volatiles liberated from the down-going slab enter the overlying mantle, lower the melting temperature of the rock and lead to magma genesis. Surface observables such as magma composition, spatial distribution, volume and temperature are determined here at depth.

Seung Lee

Massachusetts Institute of Technology
Mechanical Engineering

Advisor:
Roger Kamm
Practicum:
Pacific Northwest National Laboratory
Contact:
selee@mit.edu
Notable:
Selected as a Gates Millennium Scholar scholarship recipient.
Research Synopsis:
My research area is molecular biology using computational tools. Because of not-too-strong credibility of molecular dynamics (MD) results of macromolecules, the challenge is to ask the right kind of questions that can be answered precisely from the MD simulations. Our attempt is to design the study based on published experimental results or to coordinate the study with other students doing experiments in our group, and work cooperatively. One of our current projects is studying the interaction between vinculin and talin.

Mary Ann Leung

University of Washington
Theoretical Physical Chemistry

Advisor:
William Reinhardt
Practicum:
Lawrence Berkeley National Laboratory
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mleung@u.washington.edu
Notable:
Awarded the Klaus A. and Mary Ann D. Saegebarth Graduate Student Fellowship by the University of Washington.
Research Synopsis:
My research involves the investigation of BECs and quantum information science through analytical and computational studies. This includes utilizing numeric and visual techniques and is centered on developing theoretical and computer models.

Randall McDermott

University of Utah
Chemical Engineering

Advisor:
Philip Smith
Practicum:
Sandia National Laboratories – California
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randy@crsim.utah.edu
Notable:
Invited to and attended the 2002 Noble Laureate Conference in Lindau, Germany. Named as a John Zink fellow for outstanding work in combustion.
Research Synopsis:
Advances in computational science fall into three categories: (1) hardware improvements, (2) improved algorithms and numerical procedures, (3) improved subgrid-scale (sgs) models. It is essential that the community realize that none of these components is any more important than the others. The problems of the 21st century are simply too massive, with important physics distributed over a broad range of length and time scales, to ever hope to be solved by brute force calculation alone. My research focuses on improved sgs models for turbulent reacting flows.

Matthew McNenly

University of Michigan
Aerospace Engineering

Advisor:
Iain Boyd
Practicum:
Sandia National Laboratories – New Mexico
Contact:
mcnenly@engin.umich.edu
Research Synopsis:
Fluidic MEMS development suffers from a lack of accurate and efficient computational methods to simulate flows at this scale. Current MEMS revenue is in the billions, and fluidic MEMS offer enticing future applications like microscopic squadrons of spy planes, and bloodstream armadas of disease fighters. However, machines on the micron scale typically operate in the slip-transition regime of fluid flow, which means traditional aerodynamic tools are inaccurate. An insufficient number of particle collisions occurring at the surface of a micro-machine cause the continuum-based Navier-Stokes equations to fail. The particle behavior of these rarefied flows is accurately modeled in the direct simulation Monte Carlo (DSMC) method, but for MEMS flows, we are faced with solution times on the order of the human life span. Avoiding numerical solution is not practical either. The physics behind the phenomena at this scale are not completely understood, and experimental testing of fluidic MEMS is still under development and has a much higher overhead cost than computational research. Rapid development of fluidic MEMS is impossible unless strides are made in all of these areas. I will focus my Ph.D. research on developing the innovative numerical methods and high-performance computation necessary to provide the most cost-effective resources for future MEMS design.

Julian Mintseris
Boston University
Bioinformatics

Advisor:
Zhiping Weng
Practicum:
Lawrence Berkeley National Laboratory
Contact:
julianm@bu.edu
Research Synopsis:
Recent advances in high-throughput molecular biology, specifically genomics and proteomics, have brought about revolutionary approaches to biological science. It is clear not only that we can and should study molecular biology on this higher level, but also that computational science is indispensable in this approach, in order to deal with the amount of data that is becoming available. One area where data are becoming rapidly available is protein structure. Structrual genomics projects around the world are developing ways to crystallize proteins faster, and these crystal structures add greatly to our understanding of biology at the atomic and molecular levels.

Elijah Newren
University of Utah
Mathematics

Advisor:
Aaron Fogelson
Practicum:
Lawrence Livermore National Laboratory
Contact:
newren@math.utah.edu
Research Synopsis:
I am interested in computational biofluid dynamics and simulation of medically-important blood flow phenomena, such as blood clotting or the breakup of red blood cells (hemolysis) in flows within biomedical devices. Better understanding of blood clotting will aid in preventing clots in the coronary or cerebral arteries, thus reducing the number of heart attacks and strokes. Hemolysis has many serious side effects, ranging from anemia in patients using blood-contacting biomedical devices to distortion of blood test results that can significantly impact diagnosis and treatment.

Christopher Rinderspacher
University of Georgia
Chemistry

Advisor:
Henry Schaefer
Practicum:
Sandia National Laboratories – California
Contact:
crinders@chem.uga.edu
Research Synopsis:
My professional interests lie with computational chemistry, where one of the most promising, entirely new approaches is geminal functional theory (GFT).

Samuel Schofield
University of Arizona
Applied Mathematics

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Juan Restrepo
Practicum:
Argonne National Laboratory
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sschofie@u.arizona.edu
Research Synopsis:
My research interests are in applied geophysical modeling and simulation. This involves utilizing advanced computational techniques for petroleum reservoir evaluation, characterization, and modeling. Evaluation of existing and potential reservoirs will become vital to satisfying the energy needs of the United States. These energy resources will be of fundamental importance in national security. However, the location of the potential reserves and the risk and expense involved in developing these resources have necessitated the development of advanced computational techniques for reservoir evaluation and specifically, seismic data processing. With the aid of sophisticated algorithms and visualization systems, the risk associated with drilling can be reduced.

Matthew Wolinsky
Duke University
Geomorphology

Advisor:
Lincoln Pratson
Practicum:
Oak Ridge National Laboratory
Contact:
maw@duke.edu
Research Synopsis:
My research focuses on stratigraphic evolution in passive (continental) margin basins (e.g., offshore US east coast). Complex stratigraphy forms in response to variations in sediment transport processes driven by sea level variations over geologic time. Basinward decline in transport "energy" produces distinct boundaries between depositional environments (e.g., shoreline/shelf-break for sand/mud), where deposition is concentrated, and simulation of stratigraphic evolution over long timescales must account for movement of these boundaries. Since most sediment transport models are aimed at much shorter event timescales (e.g., a single storm or flood), models must be scaled up to compute effective sedimentation/erosion rates over stratigraphic timescales.

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