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An Enlightening Experience

THE DEPARTMENT OF ENERGY

Computational Science Graduate Fellowship (DOE CSGF) program is one of a kind. This program not only requires a broad Program of Study that branches across three major disciplines (science, engineering, applied mathematics, and computer science) and offers generous support to its participants, but it also provides the opportunity to work in a DOE national laboratory on a three-month practicum assignment.

The practicum is designed not only to complement the fellows’ research efforts, but also to expose fellows to the exciting world of ideas and scientific research that is happening in our nation’s labs.

Two bright stars in the DOE CSGF program, Diem-Phuong Nguyen and Benjamin Keen, happened upon the excitement happening in our nation’s labs.

That chance has paid off for both of these fellows, who were selected from a highly competitive pool of candidates and have gone on to become bright stars in the program. Having no experience in or with the DOE labs, Ben and Diem weren’t sure what to expect when it came time to complete their respective practicums. But, after 12 weeks of living, learning, and lighting it up in the labs, they both became respected collaborators and found themselves right at home.

Better known as ASCI, “Philip Smith (chairman of Utah’s chemical and fuels engineering department) was the speaker. He went through some sophisticated combustion simulations, and I was hooked. I didn’t anticipate any of this.”

Nguyen’s group, Combustion and Reaction Simulations (CRSIM), headed by Smith, is developing software that simulates large-scale so-called pool fires of up to 20 meters in diameter. CRSIM belongs to a larger group, Center for the Simulation of Accidental Fires and Explosions (CSAFE), which simulates high-energy explosions. CSAFE is one of four university-based centers that are part of ARL, funded by the Department of Energy.

“With a fire scenario, she says, “say jet fuel catches on fire. We simulate that because, for obvious reasons, you can’t do it experimentally. Each explosion is different – each model has ramifications for how to design better safety systems for activities like transporting combustibles. The real concern is transportation accidents, both airline and ground, but our methods apply to forest fires, too. We work on keeping fires from spreading. We can design facilities better by putting up barriers that redirect fires from what we’re trying to protect — if we know how they spread.”

That’s a big ‘IF’ Combustion is a complex process of fluid flow dynamics, fire structure, turbulence and other physics combined with thousands of chemical reactions. As much progress as there has been in numerically simulating accidental fires and explosions, no one has come up with a reliable way to calculate both the turbulent conditions inside and surrounding an inferno and the fire’s complex chemistry, involving as many as 200 species of highly reactive atoms called free radicals. Free radicals up the master chain reactions that characterize combustion, converting fuel and oxygen into other gases and, not least, soot.

“Soot is an integral part of all fires, even jet fuel, because the soot radiates and strongly affects the temperatures and pollutants coming off from the fire,” Nguyen says. “Remember that luminous fireball and the billowing black cloud of smoke during the aircraft explosion and fire on September 11? Both contain large amounts of soot. The luminous part is the soot particles radiating; smoke comes when the soot particles have cooled down.”

Modeling Fire Leads to Exciting Research

DIEM-PHUONG NGUYEN

University of Utah - Lawrence Livermore National Laboratory

Story by William J. Carnes

Anyone who missed the movie Real 8or need only turn on the nightly news for a reminder of how unpredictable and unforseen fires can be. Our collective horror has been kindled by images of Colorado, Arizona and other Western states burning and by stories of terrorists’ bombs calculated to inflict maximum damage.

All of this has stoked a sense of urgency among combustion researchers, who have spent years studying the fundamentals of explosions and the path of fire. Diem-Phuong Nguyen’s interest in the behavior of fire was sparked somewhat late, during a lecture in graduate school.

“I was in chemical engineering, just kind of hanging around,” says Nguyen, who is finishing her doctorate this year at the University of Utah in Salt Lake City, “I really didn’t have a research project. Then I went and heard a talk about the Accelerated Strategic Computing Initiative.”

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For over 10 years, the DOE CSGF program has encouraged the training of computational scientists by providing financial support to some of the most talented graduate students in the nation. Phase II for the fellowship appeared in the National Science Foundation’s Division of Mathematical Sciences publication Mathematics and Science.

DOE CSGF Fellows

DOE CSGF program work in a Department of Energy laboratory.

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

Prior to the third year of the fellowship, fellows must complete a practicum assignment at a Department of Energy laboratory. Currently, approximately 20-30% of graduate students from the DOE CSGF program work in a Department of Energy laboratory.

The disciplines pursued by the fellows involved in the DOE CSGF study a wide variety of 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, biostatistics, aerothermal engineering, chemical engineering, robotics, computational chemistry, and computational mechanics.

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.

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The most valuable part of a practicum in computational science shares a term from computing but has nothing to do with any particular computational apparatus: networking. Nguyen says, “It’s a great exposure to the scientific community, to other minds, to people who have ideas that are different from yours. People working in the combustion community have different points of view. The practicum fosters new creative thinking, it’s an ongoing education.”

And possibly “a little scary.” Nguyen continues, “Honestly, some of the ideas that are different from what the industrial scientists aren’t overwhelming and impressive enough, the labs often bring in special guest, famous Nobel laureates. I got to meet Edward Teller...”

Would she do it again? Yes, definitely. And literally. “The first experience was so positive, I went back for a second one.” To avoid being tied to one computational flow code, she spent her second summer testing her subgroup reactions models and coupling them to codes developed at Livermore. “Our group has had a dozen DOE GSFF graduate students work with us during the summer over the past four to five years, and we have found that they are all very good and enthusiastic,” says William Hamrick, a Lawrence Livermore applied mathematician and Nguyen’s practicum adviser.

What about a third practicum for Nguyen? No — as much as she would have liked another, she is too busy finishing up her degree. But she hopes that she is not finished with the national labs.

Before her practicum experiences, she hadn’t really considered a career at a national lab. The whole idea of working at a government lab sounded dull, programmed, one-dimensional. “But I found it was such an open community, with everyone encouraging you and great resources, which include not only the equipment but also the people.”

To which she adds, without pause, “I would be interested in working at a national lab. Unlike a university, you don’t have to worry about teaching, I know now that I want to concentrate on research.”

A Computational Toolbox

KEEN 2001 at Gsi vector box builds a long way towards making him “a very striking physical presence,” says Phil Colella, a segmentor at Lawrence Berkeley National Laboratory (LBNL), as he describes Ben Keen. Keen, a 24-year-old student in mathematics at the University of Michigan, spent the summer of 2001 working in Colella’s lab in Berkeley, California, while fulfilling the practicum requirement of his DOE Computational Science Graduate Fellowship.

In keeping with his physical appearance, Keen also has a “striking and confident personality,” says Colella, who served as Keen’s practicum advisor. This self-assurance allowed Keen to interact with the other scientists in Colella’s group just as thought he were one of them, “It’s unusual for someone his age, and at his point in their career,” said Colella. “He behaved as a peer of the others in the group.” As for his part, Keen clearly enjoyed being at LBNL. “It’s a nice collegial atmosphere,” he says. “Very supportive, exactly that you’re not at a university.”

The Applied Numerical Algorithms Group at Lawrence Berkeley National Laboratory has developed a suite of adaptive mesh refinement (AMR) tools for solving problems involving partial differential equations. This image shows how this AMR tool, Chombo, has been used to solve a Poisson problem and visualize the results. Such a problem may involve determining the equilibrium state of electrical fields or temperature distributions.

“Even though those are very different applications, the underlying mathematics is very similar.”

The algorithm that the algorithm has no name of its own may be indicative of the fact that algorithms do not seem to get their due when credit is distrubed up for the ongoing massive leaps in computer power and speed. “In the last 10 years a lot of people have come up with really excellent algorithms that are every bit as responsible as [improved hardware] for increasing computer speed,” says Keen. Yet they get little credit.

“...It would be too strong to say that algorithms get zero credit among those who know, but certainly to the general public, the idea is that the ‘big computers’ are the big win — but it’s really the ‘smart algorithms.’ It’s not increasing computer speed so much as allowing people to do larger simulations faster,” he says.

A Mathematical Middleman

The algorithm that Keen was helping perfect during his practicum relates to work being done to represent complex boundaries in geometry. “Things like the interior of a cylinder in an automobile engine,” says Colella.

While the representation of the boundaries is a separate effort, it can be analogized to the creation of a worty shaped cake pan.

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A theoretical chemist might come up with a new system of endowing a compound. The purely practical person would be the chemical engineer who looks at making a million pounds of this for the lowest possible cost with the minimal amount of waste.

“But, there’s a process chemist who stands between these two chemists.”

Of Water and Air

In 1998, Keen graduated summa cum laude from the University of Southern California and took up residence at University of Michigan, where he had been awarded a Regents Scholarship to pursue a PhD in mathematics and computational science, which he hopes to receive in 2003. On the way, he has picked up a Regents Scholarship to pursue a PhD in mathematics and computational science, which he hopes to receive in 2003. During his 12-week stay at LBNL, Keen found that as an ‘outside living in the house’ of the LBNL researchers who created the algorithm, he was able to bring a fresh perspective to their work and turn up several problems in the software.

The Fellowship

Keen has been recommended for the DOE Computational Science Graduate Fellowship (DOE CSGF) in late 1999, at the suggestion of Robert Keeny, a faculty member in the University of Michigan mathematics department. “I really didn’t expect to get it,” he says, “but it seemed worth a shot.”

While Keen found the application process straightforward, he did find the requirement that he fill out a professional function as an applied mathematician will require working closely with engineers. “I’ve got to be able to speak to engineers,” he says, “so I can’t just take math classes.”

Keen found his practicum match through his University of Michigan academic advisor, Smadar Karni, who introduced Keen to Colella to speak at a conference she had organized. Having been involved in the DOE Computational Science Fellowship, Keen applied for the DOE Fellowship. He says, “It’s not that I had anything to offer concerning the architecture, etc., but just that ‘hey, here’s an outside user fitting a number of the qualities of the eventual users of this software’ — the things that I find difficult/ confusing others might too, and the capabilities that I might want in part of implementing this algorithm might be things that other folks need too.

Despite Keen’s modesty, Colella points out that the kind of work he did during his practicum is particularly difficult because it deals with reconciling the ideal circumstances of mathematical theory with the imperfect world of mechanical systems.

And even though Keen finished his practicum in 2001, he continues to serve as a consultant to Colella’s group. Members will, on occasion, send e-mail messages to him asking what he thinks of an issue, such as how errors are reported to users. And, says Colella, “Even though he’s in Michigan, and has other things on his mind, he responds in a very thoughtful way.”

Keen also hopes to use Chombo in his own research. “It’s really useful to be able to make use of this tool,” he notes.

Undoubtedly the highest compliment of all came from Dr. Colella, who was asked if he would hire Keen as a full-time member of his group. “Wouldn’t hesitate for a second,” he shot back, even before the question was complete.
To determine that the universe is expanding at an accelerating rate, using dozens of lines. Each line represents an atomic combination of millions of spectral lines. Each line is a tiny piece of the puzzle, and together they form a picture of the universe’s expansion. The models are telling us that if these parameters change then we’ll expect to see this signal,” says Nugent.

This joint observational and computational modeling approach has already led to what the journal Science called the “Breakthrough of the Year for 1998.” Using dozens of supernovae at distances greater than four billion light years, the SCP and its competitors, the High-Z Supernova Search Team, were able to determine that the universe is expanding at an accelerating rate.

It’s an observation that implies the existence of a mysterious, anti-gravity property of space called “dark energy.”

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Stephan’s Quintet, the realm of the mind-numbingly large and complex.

In short, it’s a job for a supercomputer.

Modeling the spectrum of a Type Ia supernova means recreating a combination of millions of spectral lines. Each line represents an atomic type within the exploding star’s rapidly evolving atmosphere. These include silicon and silicon, with hundreds of thousands of lines representing iron in various transition states. The spectral lines are in turn strongly dependent on temperature and density in the various zones of the star’s atmosphere.

Mimicking the observational data, the models began at about one second after ignition and continue to 20 days, at which time the supernova reaches peak brightness.

“There’s a great synergy between observations and theory in this field. For me it’s a very exciting one because there’s a lot of contact between the theorists and the observers. What we do with the modeling is create a theoretical spectrum and then compare that model with observed data. We then frame questions in ways that people can do data analysis and say, ‘These models are telling us that if these parameters change then we’ll expect to see this signal,’” says Nugent.

This confluence of theoretical and technological advances led to the creation of the Supernova Cosmology Project (SCP), led by Saul Perlmutter of Berkeley Lab’s physics division. The project’s goal is to use high-redshift Type Ia supernovae in exploring a bevy of cosmological questions. The group pioneered the automatic detection of supernovae through using CDSs.

A staff scientist with NERSC’s scientific computing group, Nugent is at the forefront of a new realm of supercomputer-based computational astrophysics. He grew up looking at the stars in his Easton, Pennsylvania, backyard through a Newtonian telescope given to him by his grandfather. Now he creates it.

When I graduated, the Project didn’t have anyone to interpret their data and push the envelope by suggesting better ways to take measurements,” says Nugent, who was hired as the Project’s first theoretician, starting out as a post-doctoral researcher in Berkeley Lab’s physics division.

“The Dawn of a New Era of Supernova Science

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Modeling the Insanely Big

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Moving to 3-D

Until recently, his supernova models were created in a dimension. Now the work is about to get a lot harder.

“We’re just about to go to 3-D with our code, and this will cube the time and memory requirements and exhaust the amount of computing time I have to run a couple of simulations. So I want to make sure I’m doing this in the best possible fashion,” Nugent says.

The move to 3-D models is part of the SCP’s efforts to move beyond scientific analyses to gain even more detailed understanding of these stars’ behavior.

One key element of this is study of the polarization spectra. As Nugent puts it, when a Type Ia explodes, it is as ifphoton is coming through a polarizer, and there is the possibility of different polarization angles. At some point we are going to get simulations that will take days to run and we may want to go into the middle of a simulation and look at the data in a visual way, and ask: ‘Is this going anywhere near the result that we want?’ And if not, let’s just stop it right now and start down another path, so we don’t waste all our time on the supercomputer.” So they would help interact with the supercomputer,” says Nugent.

The role of computational supernova simulations will be increasingly important as the SCP moves into its next goal: SNAP — the SupraNova Acceleration Probe. This multi-agency, multi-institutional project, led by the National Aeronautics and Space Administration and backed by DOE’s Office of Science, will use dynamic allocation of the processors for on-the-fly realization of the computationally intensive tasks.

“Even if the most distant groundbreaking telescopes — such as the Keck 10-meter telescope in Hawaii — currently used to detect and take high-resolution spectra — SNAP will be able to detect and take spectra of faint light (especially in the infrared) from the most distant and ancient high-redshift supernovae,” Nugent says.

Even with this computational workload, there’s still the question of how to best divide up the atmosphere to maximize the computational efficiency.

you could have a very low-density chunk of your atmosphere where there are very few interactions. So if a photon comes in, it barely leaves immediately, you do very little with it. So you’d like to have just a few processors handle all those parts of the atmosphere, he says. Nugent is working with NERSC’s computational scientist Omar Marques and Tony Drummond to assess questions of load balancing, as well as exploring ways to use dynamic allocation of the processors for on-the-fly realization of the computationally intensive tasks.

“Dynamic realignment could play a particularly important role when it comes to creating 3-D models. Nugent is collaborating with NERSC’s science visualization staff to refine both the processing and data representation of these models.

“With more than 3,000 processors, NERSC’s IBM RS/6000 SP is ideal for this model. The advantage of this approach is also motivated — to use the current high-end facilities to reach a significant result. "The move to 3-D models is part of the SCP’s efforts to move beyond scientific analyses to gain even more detailed understanding of these stars’ behavior. 

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Simulating the Ultrasmall

To maximize the stockpile's ability to discourage attacks by enemies, particularly in these troubled times, engineers must ensure that the weapons remain in reliable working condition. They must also refresh them continually to incorporate the latest technological advances.

Those tasks face a key limitation. Like a majority of other nuclear nations, the United States refuses to test its weapons directly by exploding them in the atmosphere or underground. So the guardians of the stockpile – most of them in the Department of Energy's national laboratories – are placing greater reliance on simulation techniques to keep the weapons up to date.

The Microsystems and Engineering Sciences Applications (MESA) project at Sandia National Laboratories in Albuquerque, New Mexico, is designed to provide a critical element of such simulation work. It will facilitate the design, production, and testing of weapons components called microsystems. “Integrated microsystems will streamline the number of weapons components, reduce production maintenance costs, and minimize the number of fault points in the weapons system,” explains Sandia scientist Rodney Schmidt.

Schmidt has particular interest in one facet of microsystems known as MEMS, for microelectromechanical systems. These are gears, motors, sensors, and other parts no larger than grains of pollen made entirely from the silicon compounds used in computer chips and integrated circuits. They have potential uses in fields as diverse as consumer electronics and medicine.

Sandia has developed pioneering technologies that enable the production, on computer chips, of intelligent MEMS systems that know where they are and what is happening around them. This work, says Schmidt, “is an important element of our stewardship over maintaining the continued safety, security, and reliability of the stockpile.”

Not only are MEMS components minuscule in size, but many of them have extremely complex shapes. So it’s no surprise that designing and fabricating the parts can present extraordinary challenges.

The Power of Computer Simulation

Experiments in fabrication facilities to test the design of MEMS devices are a big problem because good measurements are very difficult to make at extremely small scales; the experiments typically require a long lead time to set up and conduct, and as a result the tests cost a great deal of money. Fortunately, a cheaper alternative is emerging: using computers to simulate design and performance.

That’s where people like Schmidt come in. A leader of a Sandia project called Computational Technology for MEMS, he works closely with MEMS scientists and engineers to determine how computer simulation can best help them. The project is part of Sandia's Science-based Modeling and Simulation Roadmap for MEMS, an effort that aims to coordinate and tie together all the different types of MEMS computational work needed at Sandia.

“The MEMS project is part of the MESA vision, recognizing that Sandia's computer science center needs to be active in contributing to the MEMS work and to satisfy the computational needs of the people in the MEMS center,” Schmidt explains. “Computations has become an essential element in our vision of the national laboratories. We believe that the development and application of computational tools in support of MEMS R&D is fundamental to advancing the state of the art in MEMS design, fabrication, and performance analysis. We expect that computational tools will impact all aspects of MEMS work at Sandia in the future.”

What specific mission does Schmidt’s group have? “Our goal is to identify and develop the computational tools, algorithms, and models most important to making simulation a key element of Sandia’s MEMS R&D program,” he explains. “Integrated microsystems will streamline the number of weapons components, reduce production maintenance costs, and minimize the number of fault points in the weapons system.”

Fabrication and Design Challenges

Many of the microfabrication technologies used to produce MEMS devices stem from the techniques that the microelectronics industry has developed to create electronic semiconductor devices. The three dominant technologies are surface micromachining, bulk micromachining, and LIGA. Surface micromachining forms 3-dimensional structures by deposition on and etching of thin films. Careful construction of the lithographic masks that control these steps and the application of a final selective “release” etch permits the creation of complicated free-standing movable parts.

Bulk micromachining, using chemical etching (using various acids or hydride mixtures) and dry etching (using highly directional plasma techniques) allow deep, high aspect ratio features to be scalped into the bulk of materials such as silicon, quartz, and glass. LIGA, jokingly referred to as Long Incomprehensible German Acronym, stands for Lithographic Galvanomforming und Abformung, or lithography, electroplating, and molding. The process forms small 3D structures by mold fabrication followed by electro-deposition.
To create more effective and more complex MEMS, designers must incorporate an increasing number of process steps and material layers into the fabrication processes. For example, in surface micromachining, the current standard at Sandia is a process known as MUMMKT (for Sandia Ultra-Planar Multilevel MEMS Technology) which, after several hundred different steps, yields a 5 distinguish isolation levels. Designing a part for manufacture with this process requires more than defining the final geometry directly. Rather, a designer must create a set of up to 14 two-dimensional lithographic masks that combined with the specifics of the process, create the final MEMS product. Not surprisingly, this indirect method of designing parts presents a challenge that becomes more difficult, time consuming, and subject to error as the complexities of the parts and processes increase.

These difficulties make the use of automated and fast design tools essential. Of particular importance is the ability to automatically generate an accurate 3-D solid body representations of the MEMS device that will result from a particular set of 2-D masks. Designers can then visualize evaluate and numerically analyze the solid model for correctness. Working with a model in this way improves designers’ ability to recognize problems and achieve early success with production.

Developing Collaboration

The MEMS technology team doesn’t work alone on its projects. “As a group doing applied research we bridge the gap between the ground-breaking work of computer scientists and applied mathematicians working on massively parallel computer systems and the applied engineers and scientists who have real-life problems that need solutions today.” Right now we’re working closely with the people who are designing the surface micromachining area. One of our goals is to further develop collaboration with fabrication specialists,” Schmidt explains. “One of our projects involves working closely with surface chemists to understand better the detailed physics associated with the etching and deposition processes. We have to understand their problems and they have to understand what we can do so that together we can come up with the best solutions. We have to work together.”

The group also has access to the powerful computing facilities of the national laboratory, as well as to a host of world-class specialists in computational mathematics, algorithms, and parallel computing. “Sandia brings the ability to leverage massively parallel computing to solve challenges of this type,” Schmidt says. “Some of the things we can do are unique. The national labs have particular strengths, including large numbers of talented people who can collaborate in an environment in which different people can provide diverse resources in an interdisciplinary situation.”

Challenging technical problems of national importance, state of the art computational resources, and the applied engineers and scientists who have real-life problems that need solutions today. Right now we’re working closely with the people who are designing the surface micromachining area. One of our goals is to further develop collaboration with fabrication specialists,” Schmidt explains. “One of our projects involves working closely with surface chemists to understand better the detailed physics associated with the etching and deposition processes. We have to understand their problems and they have to understand what we can do so that together we can come up with the best solutions. We have to work together.”

The MESS program has already signed up its first DOE CGSF fellow. Matthew J. McNerth from the University of Michigan is a student who will spend the summer of 2002 working with staff member Michael McGlinch in the Noncontinuum Transport and Micromach Science Department.

Exciting Opportunity

How did Schmidt get into this line of work? “My manager invited me to lead the project when it was initiated,” he recalls, noting that he hadn’t been an expert in MEMS up to the time of his selection. He had previously carried out applied research in two main areas: modeling turbulent reacting flow and developing computer codes to simulate the physics of severe accidents in nuclear reactors. The fact that he is now working on computer simulations for MEMS, he says, “reflects the Sandia environment. You can work in an area for five or six years and then move to something different and exciting when the opportunity arises.”

His team doesn’t work in isolation at the Lab. Members frequently collaborate with scientists in industry. “That benefits everyone involved. To show that components going into weapons are safe and reliable, we need broad experience of how they perform in a range of environments,” Schmidt explains. “Incorporating the components in commercial items unrelated to nuclear weapons is thus important to obtaining that experience. This helps us to understand that the fundamental technology is working reliably.”

The computational tools and techniques that Schmidt’s group is developing have broad potential application and will help to stimulate applications of the technology in civilian areas. For example, one promising field is MEMS, a technology that will lead to products such as biosensors, microphones, and microchips on chips with direct applications in medicine. As Schmidt explains, “All of us at the lab recognize and appreciate that the technology being developed in support of national security concerns often has spin-offs into a wide range of non-defense related areas that can have a direct impact on improving our quality of life.”

Schmidt’s group is currently working on line distinct tasks that focus on different computational problems. They are:

> A 3-D parallel process geometry modeler

This is a computer code written for multiple central processing units that automatically converts design layouts of two-dimensional masks into solid body representations of the three-dimensional components that the masks will produce. The goal is to provide fast, accurate, and robust simulations that will permit designers to recognize and correct potential design problems.

> A ‘post-a-nit’ MEMS design tool

This project aims to revolutionize the design of surface micromachining parts by allowing the designer to create 3-D designs directly, without having to define 2-D masks. Schmidt’s group is developing algorithms and computer software that will automatically generate the 2-D mask sets and the tool layout represented by the designer.

> A level-set based feature scaling code

Many researchers create fundamental aspects of the surface chemistry at the extremely small scales of MEMS devices during etching and deposition. This work, called CHSFLs, for Chemically Induced Surface Evolution with Level-Set, tracks the evolving surface topology while simultane-

ously modeling the complex surface chemistry that drives the process.

> A MEMS specific modeling environment

To analyze and test the performance and behavior of a new MEMS design, a computational model that represents the design in complex geometry must be generated. However, accurate results depend strongly upon the quality of the mesh used in the simulation. This work is developing new algorithms for automatically generating high quality meshes.

> Molecular dynamics for LISA

This effort seeks to explore the viability of using what is called “molecular dynamics simulations” to understand better the physical processes that control the dissolution of polymers.
Future Climate

"IT’S ALWAYS BEEN THE CASE" that the people with the largest computer have been able to produce the best weather forecasts," says John Drake, speaking on the phone from his office at the Department of Energy’s Oak Ridge National Laboratory in Tennessee.

He’s been listening intently to weather forecasts for the past several weeks. The southeastern seaboard has been inundated with heavy late-winter rains. Yet, beyond the immediate question of whether he should be wearing hip waders to work, weather forecasts are small computational potatoes to this computer scientist and climate modeler. While a long-range weather forecast is seven days, Drake’s pioneering parallel supercomputer climate models are currently pushing out forecasts for the next two centuries.

These parallel climate models developed by Drake, in close collaboration with climatologists from the National Center for Atmospheric Research (NCAR), in Boulder, Colorado, and other national labs, are providing an unprecedented peak at the fine details of future climates. This supercomputer-generated information isn’t just about global temperatures, but increasingly about regional details, such as the mean temperature in central Iowa in 2075. It’s crucial climate forecasting that is helping inform Iowa in 2075. It’s been listening intently to weather forecasts for the past several weeks. The southeastern seaboard has been inundated with heavy late-winter rains. Yet, beyond the immediate question of whether he should be wearing hip waders to work, weather forecasts are small computational potatoes to this computer scientist and climate modeler. While a long-range weather forecast is seven days, Drake’s pioneering parallel supercomputer climate models are currently pushing out forecasts for the next two centuries.

The Parallel Supercomputers that Could

In the late 1980s, Drake’s background in applied mathematics with a focus on computationally demanding fluid dynamics problems made him the perfect candidate to work in the quickly developing field of climate modeling.

"Climate is the granddaddy of fluids problems. The general circulation of the atmosphere and the oceans are fluids problems," notes Drake, now the Computational Climate Dynamics Group Leader at Oak Ridge.

However, it is a problem that severely outpaced the computing power of the day. The climate models of ten years ago were simplistic by the standards of today. That’s because people didn’t know what to put in them. They just couldn’t afford to do the computation. So they made simpler models," recalls Drake. "In the last three to four years we’ve gone from having the power only to simulate the atmosphere in a climate setting to being able to create coupled general circulation models, ones that combine the atmosphere with ocean, sea ice and land surfaces. That’s a big change in complexity and our understanding of what constitutes climate."

Back in the dome days of the Internet, the challenge of producing better climate models pushed Drake and his colleagues to explore a new computational approach — massively parallel computers.

"This was in about 1989, just when early Intel chips were getting cheap and it became obvious that you could string a lot of these together and compete with a supercomputer," Drake says.

At the time, notes Drake, massively parallel computers were largely a computer-science novelty to climatologists. Most were accustomed to running sophisticated vector-based models on CRAYs (though some of these models, including a pioneering one at NCAR, were parallel vector applications). But to Drake — working at the borders of mathematics, supercomputing and climatology — distributed-memory massively parallel systems offered an intriguing advantage: their structure mimicked the highly interactive nature of climate.

"The realization with massively parallel computing was that if you had lots of computer chips you could break a calculation up into several pieces. You could divide and conquer. So instead of one long vector, you had a bunch of short vectors, and the memory is spread out," recalls Drake. His Oak Ridge lab had one of the first of what he calls "toy" massively parallel computers.

However, the distributed-memory architecture of parallel computers also presented a major new problem. How would climate models deal effectively with message passing, the sharing of information between processors? After all, when processors are sharing information they’re not performing calculations.

In the early 1990s, the DOE created the CHAMMP (Computer Hardware, Advanced Mathematics, and Model Physics) program to directly address this problem. The program was a collaboration between some of the top computational scientists at DOE’s Oak Ridge and Argonne National Laboratories, and climatologists from the NCAR.

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"Climate is the granddaddy of fluids problems. The general circulation of the atmosphere and the oceans are fluids problems."
John Drake received his PhD in mathematics from the University of Tennessee in 1991. Since 1999 he has been the Group Leader of the Climate Dynamics Group in the Computational Sciences Section at Oak Ridge National Laboratory. His current research interests include numerical methods and parallel algorithms for climate dynamics, numerical solution of partial differential equations and integral equations, with particular regard to supercomputing applications.

Further Reading


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The lock-step march of advances in computational and climate science is now presenting a whole new palette of problems for climate modelers. Call it the “more” factor.

The “More” Challenge

The lock-step march of advances in computational and climate science is now presenting a whole new palette of problems for climate modelers. Call it the “more” factor. Climate modelers like Drake are faced with not only new data, new complex climate models and ever more intricate parallel computing hardware. It’s a phenomenon that’s forcing a greater-than-ever level of interdisciplinary collaboration in developing climate simulations.

There are two main competing approaches: grid point approximations and transform methods. While transform methods are the traditional approach to climate models, the grid point method is more computationally efficient, since it relies on more local mathematics. Drake, an advocate of the transform method, counters that speed isn’t everything. The two methods have their differences in the results they produce.

“There was a ‘bake-off’ last year; we did evaluations of three different algorithms, composing a grid point model with two versions of transform models, all of which had had significant investment to make parallel algorithms. The chemists like one and the meteorologists like another,” Drake says.

For example, tropical regions are better represented with the transform model, while the grid point model more faithfully conserves atmospheric chemistry, making it chemists’ preferred choice. One solution that Drake and others are exploring is to combine the best elements of both approaches with focus grid transform models.

The combination of more complex hardware architecture and more complex models is also spurring Drake and Malone’s team to grapple with software development issues. These are particularly relevant for recent global coupled models. These models integrate the climatic roles of atmosphere, oceans, sea ice, land surfaces and, increasingly, other factors such as volcanic activity and solar variability.

“One of the things that we’ve tried to do recently is bring modern software practices into this situation,” says Drake. “It used to be that the problems were small enough, and the codes were simple enough, that individual scientists could in fact know everything that’s in the code. But now with this complexity that’s no longer the case. You really have to work in teams.

Addressing the triumvirate of “more” problems holds the promise of opening the way for the next generation of climate simulations, once that will provide ever greater accuracy and resolution.

The accuracy of global climate models is a major scientific — not to mention political — issue. Using a parallel climate model that incorporates many of Drake’s algorithms, NCI’s Warren Washington recently created a simulation of historical data (1850 to present) with a 55 percent confidence interval. Drake is now working with him to shepherd through Oak Ridge’s and NCI’s massive parallel computers what might well be the most definitive U.S. models yet for the impacts of global warming.

Unlike past simulations, Washington’s current climate forecasts are based on ensembles of multiple runs of a model. This is the way that weather forecasts are constructed. However, only in the past several years has there been the computing capacity to perform ensemble models for multi-century global circulation climate models.

Says Drake, “When people start to ask questions about the implications of climate change, one of the things they quickly get to is what’s going to happen to the rivers, vegetation, and agriculture on a local level. Not just east coast or west coast. You’d like to be able to have 30-kilometer resolution over the U.S. Currently we cannot provide that kind of information. But I’m hoping that new algorithms and increased computing power will provide a way to achieve this increased resolution and accuracy.”

Drake and others are working to improve the quality of his models for the ultimate in fluid dynamics problems.

But the question resulted in a still-simmering computational controversy over how to maximize the efficiency and accuracy of these parallel models.

Drake and others are exploring is to combine the best elements of both approaches with focus grid transform models.
Housing Lasers

In this instance, however, the venue will not be the fiery interior of a star, but the more tranquil surface of planet Earth. The specific location is the National Ignition Facility (NIF), now under construction at Lawrence Livermore National Laboratory (LLNL), Livermore, California.

The earthbound fusion process that will take place in NIF, which is scheduled for completion in 2008, has been successfully created in smaller, predecessor laser facilities at LLNL, known as SHIVA and NOVA, but more energy had to be used to create those fusion reactions than was created by them. The intent is to reverse that equation in NIF, so that the process produces more energy than it consumes. If the process is successful, nuclear fusion could provide an endless source of energy, since the fuel contained in the target capsule consists of the hydrogen isotopes deuterium and tritium, and hydrogen is the most abundant element in the universe.

Another reason for the construction of NIF falls under the heading of “stockpile stewardship,” which refers to maintaining the nation’s nuclear weapons capability. Although the Comprehensive Nuclear Test Ban Treaty has not been ratified by Congress, the U.S. has complied with the spirit of the treaty and has not tested nuclear weapons since 1992. NIF will be used to replicate the intense pressures and temperatures that occur during a nuclear explosion without creating an actual explosion.

““There’s a large effort to try to compensate for not being able to test weapons anymore by using computational methods, doing numerical simulations, as well as getting experimental information from facilities like NIF,” explains Milo Dorr, a LLNL mathematician and staff scientist.

Of X-Rays and Plasma

NIF will be used to replicate the intense pressures and temperatures that occur during a nuclear explosion without creating an actual explosion.

Of course, recreating the energy-producing process that takes place in the stars is an extremely complex process that requires, among other things, a tremendous amount of computational simulation work long before laser ever strikes target.

Complicating matters is the fact that the actual nuclear fusion process that will take place inside NIF isn’t as direct as it may seem, in that it is not the laser beams themselves that create pressure on the fuel capsule. Rather, pressure is created by X-rays that are generated when the laser beams hit the inside of the capsule, called a hohlraum, as well as the capsule.

In addition to generating X-rays, a hohlraum materials. The result is plasma, which, instead of being composed of atoms, is a mix of positively charged ions and negatively charged electrons. Such matter is found in the atmospheres of stars, and in thermonuclear reactions. Unfortunately, the plasma, in turn, can have a deleterious effect as the laser light passes through it.

Simulating Plasma and Light

That’s where Dorr and his group of mathematicians, physicists, and other scientists come in.

Among them is Jeff Hittinger, a postdoctoral fellow who received a PhD in aerospace engineering and scientific computing from the University of Michigan with the aid of a DOE Computational Science Graduate Fellowship (DOE CSF). Another DOE CSF Fellow, Edward McKay Hyde, worked on the computer simulation project at LLNL to fulfill the practicum requirement of the DOE CSF.
During his practicum at DOE's facility in Los Alamos, New Mexico, Hittinger worked on computer modeling of radiation hydrodynamics, which deals with the effects of light propagation through a fluid, such as air or a plasma, under conditions of intense radiation. Although different from the NIF project he is more engaged in, the subject is closely related. And, in fact, he obtained his postdoctoral assignment at LLNL through contacts he made while at Los Alamos.

“My group leader at Los Alamos was very active involved in the DOE CSGF program,” he said. “He and members of his research group moved from Los Alamos to Livermore and put me in contact with a member of the ALPS team, said Hittinger, using the acronym for Adaptive Plasma Laser Simulation. Simulation, the NIF project in which he and Dorr are currently involved.

Conserving Computer Power

The purpose of ALPS is to improve the efficiency of an existing computer model that simulates the complex laser/plasma interaction in the hohlraum more efficiently. Dorr hopes to accomplish this through ALPS by focusing computational power precisely where it is needed, when it is needed, rather than have the calculations look at the entire picture all of the time. Currently, modeling work is parcel out among a cluster of parallel computers that run simultaneously to solve a problem. Combined, these machines are equivalent to 512 individual workstations, and can run 860 billion multiplications per second. Such computer power doesn’t come cheap, and whatever can be done to make use more efficient is valuable.

The original laser/plasma simulation program represents segments of the hohlraum as a mathematical mesh of grids, or cells. With as many as 1,000 cells in each of 5 directions (X, Y, and Z), the box can contain up to one billion cells. Equations simulating the light and the plasma then take a numerical look at what is happening inside those cells at any given moment during the laser firing process.

While thorough, having a uniform grid system that allows examining the inside of any one of your billion cells at any time “has a certain cost to it in terms of how much memory I have to use in the computer and how long I have to run the calculation,” says Dorr. Besides, it turns out that it is not necessary to look at all the cells all of the time.

“In certain parts of the plasma there may be a lot of things going on, so I need to use a lot of grid cells in that particular area, whereas elsewhere there just isn’t that much going on at all, so I don’t need as much grid resolution,” explains Dorr. Hence, the purpose of this project is to turn that uniform grid of cells into an adaptive grid — as in the Adaptive in ALPS — that can adapt in concert with the needs of the modeling process.

“Suppose I’m only interested in something that’s going on in the middle of this rectangle. Then I don’t necessarily need such high resolution in the outer part of the rectangle,” says Dorr. “What I’d like to do instead of using one billion mesh cells everywhere, is concentrate my mesh cells in the middle of the problem where there is fine detailed features that need to be resolved, and in the outer portion of the region, where I don’t care as much about what’s going on, I could have a much coarser resolution.

The result could be the need to look at a million rather than a billion mesh cells. “The basic idea is to use the computer resolution only where you need it and, therefore, save on the total cost of the calculation.”

To verify the calculations, experiments are sometimes run at the University of Rochester’s Omega laser facility, a much smaller sibling of the trouble-making NIF. But, since there are more potential experiments to be run in Omega than time and money allow, ALPS and Omega are entering into a two-way relationship in which Omega tests ALPS calculations, and ALPS calculations help determine which experiments Omega should run.

“What we’re hoping to do is use our computational model to try to winnow out some cases, so we can tell the experimental folks. We’ve seen this behavior, these types of problems, so you may want to design an experiment in this regime. On the other hand, we ran all these other problems and nothing really showed up so you may not want to waste any time probing in that part of the parameters,” says Dorr.

Although ALPS has been an ongoing program for about three years, according to Dorr, “this is an open-ended research area. As people start doing more experiments on NIF itself, I think there will be even greater demand for computational simulation support, not only to design the experiments, but also to understand what happened when they did them. I think this is a growth area.”
Working a Beat

IN THE FALL OF 2001 an article was published in Cardiac Electrophysiology Review that summarized the current work on computer modeling of atrial fibrillation, the debilitating quivering of the heart’s upper chambers. All things being equal, there was probably about as much chance that Wonho Oh would ever see the article as that he would get hit by lightning.

By Jacob Berkowitz

DOE LAB RESEARCH
Lawrence Berkeley | Oak Ridge | Lawrence Livermore
Brookhaven | Los Alamos | Pacific Northwest | Argonne

Electrical Pump

While most of us know the heart as a pump, fewer of us think of the large, essential muscle in our chests as an electrical pump. Yet, it is electrical activity that regulates the heart’s normal, steady rhythm of between 60 and 90 contractions a minute. In a healthy heart, the cardiac rhythm originates in a small area located in the upper part of the right atrium, called the sinoatrial node. The impulses from the heart’s natural pacemaker travel as an electrical wave through the atria, and then — after a hundredth-of-a-second delay that allows blood to enter the ventricles — through the cells of the ventricles. This electrical stimulation causes the cells to contract forcefully, pumping blood through the body.

Arrhythmia occurs when, as a result of structural or dynamical problems, one of these electrical waves is locally blocked and breaks, turning the wave into a potentially deadly spiral of electrical activity.

“When these spiral waves are produced in the heart, they have a much faster frequency than your normal pacemaker,” says Fenton. “Since they rotate much faster, they take control and your heart starts pumping much faster — called tachycardia. Then the spirals tend to break into multiples. And when...
you have a few of these spirals all over your heart, each one at a very high frequency and out of phase from the others, then the whole heart is just quivering and not pumping anymore.”

About ten percent of all Americans over the age of 65 have some level of chronic atrial fibrillation, a condition that results in weakness and numerous long-term circulation problems. Ventricular fibrillation almost results in death if not treated within minutes.

**Heart Modeling**

In the early 1980s, Beth Israel Medical Center cardiologist Dr. Steven Evans began collaborating with a mathematician to numerically model the heart’s electrophysiology. In 1998, he recruited Fenton, who was then working in high-energy physics, to further pursue the computational modeling of this electrical activity.

The pursuit of heart electrophysiology modeling is driven by the fact that cardiologists are already well aware of the potential to treat arrhythmia. Patients with abnormal heart rhythms can undergo what has become a procedure known as an electrophysiology study. A catheter is inserted into a patient’s femoral vein in the groin, and then guided up into the heart. The doctor then simulates the heart with electrical signals to make it beat at normal rates and to observe any irregularities. Based on this test, the cardiologist can use a variety of drugs, surgical techniques, or a small, automatic defibrillator worn by a patient, to prevent arrhythmia or to convert irregular rhythms back to normal.

The problem is that even given these medical techniques, cardiac arrhythmias are still a major killer, and their cause and dynamics—the breaking of the electrical wave and spiral wave behavior—still remain largely a mystery.

**The Code**

Working with experimental data, Brookhaven’s Oh is methodically developing the parallel computational code and algorithms that will enable Fenton, Evans and other researchers to minutely model atrial and ventricular activity with greater precision and speed than ever previously achieved.

Initially he’s developing a three-dimensional slab model, one that still acts as a validation and testing ground for building the parallel code.

“When you simulate a part of the slab tissue, you expect a certain behavior of the electrical potentials, as seen experimentally. At this point, I have a basic set of code and I have been testing it in a serial fashion in a single processor with a small tissue sample to see whether the resulting potentials look reasonable. Qualitatively it’s working, the wave is propagating, but I still need to confirm it quantitatively,” Oh says.

After this initial phase is completed, the electrophysiologists will get what they are waiting for — movement of the model to Brookhaven’s Galaxy parallel supercomputer. The Galaxy cluster consists of 77 Premium III dual processor nodes, each with one gigabyte of memory. The nodes currently communicate through a Message Passing Interface (MPI) library, though Oh says he plans to use OpenMP format as well as MPI in the near future. (The OpenMP format allows multiple threads on a single node and eliminates unnecessary message passing between the processors on a single node.)

“The final goal is to make my code work for parallel machines so that I can get the result very quickly,” says Oh. “The real challenge is that you want to have a scalable algorithm, so that once you have numerous processors available, the computing speed grows at the same rate as the number of processors.”

**Lifesaving Knowledge**

It is this speed at the bi-domain, human ventricles or atria level that will significantly advance the theoretical understanding and, it is hoped, treatment of arrhythmia, says Fenton.

“The speed of parallel supercomputing allows for a parameter search, one that explores the whole range of possible conditions, such as ischemia (reduced blood flow) to the levels of sodium ions. You need to be able to do a lot of different simulations with many different parameters, and you can’t do it if it takes a day to do one simulation — then you don’t get anywhere.”

Getting somewhere in science is always important, but never more so than when the prospect of lifesaving knowledge is on the horizon. Sophisticated new simulations of fibrillation and arrhythmia in human hearts hold the promise of providing the in-silico processing of new anti-arrhythmia drugs, more effective defibrillation, and improved surgical techniques to treat arrhythmia.

All of this is being aided by a computer scientist who at the start of the project had to reach for a dictionary to understand cardiac terminology.

Concludes Oh, “Simulations are not going to replace experimental data. But numerical simulations are highly reproducible — they’re not dependent on the conditions present in an experiment which make it difficult to reproduce them. Once you know that what you’re simulating is identical to the experiments, then you can make more replicates and do them faster without having more problems.”

**Collaborators**

Wonho Oh received his PhD in applied mathematics from the State University of New York at Stony Brook. He is currently an Assistant Professor in the Department of Applied Mathematics and Statistics at the State University of New York at Stony Brook, as well as a Research Associate in the Center for Data Intensive Computing at Brookhaven National Laboratory.

Flavio H. Fenton received a BS degree in physics from Universidad Nacional Autonoma de Mexico (UNAM) in 1990 and MS and PhD degrees in physics from Northeastern University in 1992 and 1999, respectively. Since 1999 he has worked as a visiting medical physicist at the Heart Institute, Beth Israel Medical Center, New York. His current research interests focus on models of cardiac cellular electrical activity and computer simulations of arrhythmias.

**Publications**


You can find more information at the following websites:

- [Flavio.Fenton@hofstra.edu](mailto:Flavio.Fenton@hofstra.edu)
Attila the Code

A TEAM AT THE LOS ALAMOS National Laboratory has developed a new computer model that predicts how radiation travels through space. Potential applications range from better design of nuclear power plants to improved delivery of medical therapies.

Why Attila?

Woe the name Attila? It has nothing to do with any Hun-like characteristics of the code. “I opened my Webster’s Collegiate Dictionary, looked at names, and grabbed one that was short and easy to type,” McGhee recalls. “I started in the ‘A’s.”

One characteristic that the code shares with the notorious Hun is sheer power. It can help design “anywhere you have a radiation source,” says McGhee. “It involves a lot of physics, a lot of math, and a lot of computer science.” The code provides a complete solution of the radiation transport equations in terms of spatial dependence, angular dependence, and energy dependence. As a result it permits scientists and engineers to deal with such radiation effects as dosage rates, rates of energy transfer, the deposition of energy in two-dimensional and three-dimensional regions, and thermal loading—all issues of value in a variety of scientific and engineering applications.

How does Attila differ from other transport codes?

Attila in Action

Attila promises fruitful applications in three general fields. First is radiation transport calculation for the commercial nuclear industry. By effectively calculating the distribution of neutrons—elementary particles that are fundamental components of atomic nuclei—and gamma rays—a form of high-energy radiation—the code permits nuclear engineers to calculate the protection and shielding needed by nuclear power plants, and to check that these components of existing plants are working effectively. Similarly, Attila promises to help designers of future fusion reactors tame the power of the hydrogen bomb in entirely safe structures.

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The scientists at the national laboratory have proved just as important as equipment in helping to develop the Attila transport code most efficiently. “You start out with a graph outlining the tasks that need to be done,” explains Pautz. “None of us was familiar with graph theory. But there were people right around me whom I could ask. What otherwise might have taken weeks or months for me to solve took less than a week.”

McGhee agrees. “Theoretically we could have accomplished the work we’ve done over the Internet,” he says. “But it’s certainly a lot more convenient to have everybody colocated — to have experts ready by hand.”

The team has also taken the opportunity to expand scientific understanding. McGhee, Pautz, and Waring all have PhDs in nuclear engineering. But these days, says McGhee, “we often think of ourselves as computational physicists. There is a lot of computer science, numerical analysis, and software engineering required in addition to the knowledge of the physical processes and mathematics involved to create a simulation tool like Attila.” In Waring’s view, the national laboratory’s facilities and people, along with the cutting-edge work in transport numerical methods, present a strong attraction for scientists.

Graduate students have the opportunity to share in the excitement. In fact, a student from the University of New Mexico is already working on charged particle enhancements for Attila. That’s a significant problem because many transport codes can deal only with neutral particles such as neutrons. Plans, the work offers challenges beyond the norm.

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The body is often compared to a machine. Many scientists have liberating themselves from the metaphor in favor of fresh, raw literalism: the body is a machine. The human body is made of parts that are self-contained machines interacting with one another. Molecular-level changes lead to cellular ones; cellular to tissue, and so on to organs and organisms, providing whatever the body needs to plug along.

Designer Cells

The tiny machines and the processes by which they harness, transform and transport energy, are biochemical and molecular components from which they are built and rebuilt, the network that links them and keeps them working together, environmental insults that trigger developmental errors that cause them to fail—all follow the rules of physics and chemistry and can therefore be modeled mathematically and computationally. The real test becomes whether the cell works according to a deep whose complexity can be defined in the most efficient mathematical and computational terms possible.

The Virtual Cell Project

At the Department of Energy’s Pacific Northwest National Laboratory (PNNL) in Richland, Washington, David Dixon and his team are building what he calls the virtual cell. Under the auspices of PNNL’s Bioinformatics Systems Initiative, they are five years into an intense and massive data-churning, virtual cell initiative, they are five years into an initiative, they are five years into an intense and massive data-churning, computational biology effort to enable predictions of real cell behavior; information that may one day assist experimentalists in understanding the biochemical, crystallographic and magnetic interactions that compose a cell.

Much of what we currently know about the internal structural details of cellular machinery, proteins and DNA is based on optical imaging, other microscopic, crystallographic and nuclear magnetic resonance. For instance, the tinker-toy model of DNA’s double-helix structure arose from interpreting its crystal portrait. Today protein crystals and the amino acids and peptides from which they are made are depicted as colorful, 3D computer renderings which they are made are depicted as colorful, 3D computer renderings which they are made are depicted as colorful, 3D computer renderings which they are made are depicted as colorful, 3D computer renderings which they are made are depicted as animated and modeling effort to enable predictions of real cell behavior; information that may one day assist experimentalists in understanding the biochemical, crystallographic and magnetic interactions that compose a cell.

We “are taking advantage of all of the biological data coming in, including genomics and proteomics to identify the machinery of the cell, including proteins and protein complexes that do work in cells and pass instructions essential to life,” says Dixon, associate director for Theory, Modeling & Simulation in the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), a DOE national user facility located at PNNL.

“We want to understand the location of all these things in space and how they change in time so we can understand how the cell processes information and how it communicates with other cells.”

Cellular Simulations

The virtual-cell approach is to traditional biology as digital film is to 3D computer renderings that look like a dancer festooned with ribbons. Dixon notes that the models developed by his team are built on data gleaned from experimental biology. Experimentalists tease out a cell’s functional biology, inform models and offer a way to check a simulation’s veridictory.

The simulation adds a sort of narrative fluidity to the frozen-moment stillness of experimental results and can reveal a biology that may be invisible to experimentalists. A life-or-death bit of biology may take but a nanosecond, but it’s crucial that everything that takes place in that sequence are accounted for if a model is to prove useful.

For instance, Haluk Resat, a member of Dixon’s group, has run simulations of the signaling agent epidermal growth factor, or EGF. Cell signaling is a sort of wireless communication that controls all complex functions in the hierarchical network, from protein to cell to, in this case, skin. EGF works by binding with an EGF receptor, a portal on the cell’s membrane. This binding sets off a cascade of chemical reactions inside the cell that produce signals that make their way to the nucleus, where proteins-building genes are expressed. Resat’s model integrated what is known about how protein binds to fine-tune the cascade reaction and, in the process, to quantify not only which proteins are expressed but where inside the cell the processes that lead to protein expression occur—information that was otherwise invisible between slides in the projector.

“Because we’re running the simulations for a long time, we see different features that you would in experimental situations. The models must account for movement through time so they can predict how a cell will respond to a given perturbation and to various chemical reactions.” The resulting signals disperse throughout the cell, leading to further biochemical reactions, which can lead to proper function or to disease, depending on the nature of those reactions and where they take place.

Today protein crystals and the amino acids and peptides from which they are made are depicted as colorful, 3D computer renderings that look like a dancer festooned with ribbons—sans the dancer.
interface between the proteins in the p21ras (yellow) and RasGAP (blue) complex. Close up look at the structure of the active site where hydrolysis of GTP takes place. Part of the proteins are removed for clarity. Drawn as sticks are the GTP molecular waters involved in the hydrolytic reaction, and the important area of the complex is marked red. (a) LNRGAP (left) and RASSF1-C (right).

In a paper published last year in the *Proceedings of the National Academy of Science,* simulations by Roat, T.P. Stratanova, J. Miller, and D. Dixon, as part of the virtual cell project, pointed to a chemical reaction involving an "arginine finger" structure in a group of so-called molecular switches near membrane surfaces. The switches mediate the chemistry that regulates cell proliferation and differentiation. This protein, called Ras, is “of special interest because a mutant form of Ras is the application of numerical simulation to chemical and biological problems, with a focus on electronic structure theory. Dr. Dixon has published more than 350 papers on a wide range of topics.

"The simulations showed that biology has to conform to the rules of chemistry and physics, in that charge balance — an equal number of positive and negative charges — in the active site of the protein plays an important role," Dixon says. Without charge balance, essential chemical reactions cannot take place, and "the protein does not function properly; the switch does not work and you can get rapid cell division leading to cancer."

Their simulation suggested the arginine finger plays a role — unseen by those studying the Ras crystal structure — in refocusing reactions involving water, or hydroxide, that are displaced in the mutant forms of Ras. Their work has formed molecular biologists to look more closely at the arginine finger and offer a much more refined, alternative, experimental-based explanation of hydroxide in the Ras complex.

**Modeling Techniques**

As in digitizing visual information, data compression is a key issue in computational biology — that is, what is the least amount of information-space required to generate the smallest and most accurate and refined, mathematical model of a biological system? Dixon says. Without charge balance, essential chemical reactions cannot take place, and "the protein does not function properly; the switch does not work and you can get rapid cell division leading to cancer."

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**References**

The arginine finger of RasGAP helps Gln61 align the nucleophilic water in GAP-stimulated hydrolysis.**

"We're developing techniques that will work with a range of cells," Dixon says. Besides the work in mammalian cells discussed above, "we're also interested in modeling microbial cells as part of the DOE's Genomes to Life initiative that began with the Human Genome Project. This effort speaks directly to DOE's core missions: basic science, energy research and environmental remediation. Microbes have odd appetites, on the menu of some might be the greenhouse gas methane, or toxic metals in the ground."

"In a practical sense, we're interested in the question of how to modify parts of a cell to deal with nuclear waste — or even how to get a cell to do something," Dixon says. "You want to control cells so that they will chew up things that they should. If you want to prevent the mobility of uranium or plutonium, for example, you don't want to neutralize another metal such as chromium that makes the toxic material in the ground more mobile."

When enough simulations are run and verified by experimental data, will the result be a massive database of blueprints for recombining cells? With good chemistry and engineering it's certainly possible that whole designer cells would follow, though Dixon's group will continue to concentrate on how the cellular machineries acts and how best to modify that behavior.

"The simulations showed that biology has to conform to the rules of chemistry and physics, in that charge balance — an equal number of positive and negative charges — in the active site of the protein plays an important role."
And just as advanced technology has given new tools to those medical researchers, so too has it furthered the quest of materials scientists, primarily through the power of computer simulation.

Most of the inanimate objects in question are made of either metallic or ceramic materials, both of which are actually conglomerations of microscopic crystals. What looks like a solid aluminum spar of an aircraft wing, for example, is really a mass of microscopic crystals. And the spaces between those crystals, which are occupied by a world of rapidly moving atoms, constitute the weak links in the material. Hence, if that spar fails, it will likely crack along the boundaries between those crystals. While engineers know approximately how long that aluminum spar will last, what they don’t know is where and how it will crack. So, to prevent any untoward failure, they must redesign that spar, making it heavier than it would have to be if the reasons behind a potential failure were more fully understood. And that’s where Dieter Wolf and his colleagues at Argonne National Laboratory (ANL) come in. Wolf is a senior scientist and leader of the Interfacial Materials Group, which is responsible for developing computer simulations to learn what is going on in those spaces between the crystals.

“Material’s microstructure is what controls the properties of the material,” explains Wolf. “The nature of bonding of the atoms in individual interfaces and the entire spatial network of these grain interfaces is what controls the properties, and that’s what we try to understand by simulation.”

And because Wolf’s group uses simulation methodology that is not material specific, their work can apply to virtually everything from aircraft wings and jet engine turbine blades down to the submicroscopic features of modern electronic circuitry.

Predicting and Preventing

Two-pronged goals drive this work. One is to develop an understanding of the characteristics of materials so that engineers have a better understanding of the tolerances of the materials used in their designs. The other is to provide information that can be used to improve the characteristics of various materials for given applications during the manufacturing process.

An engine’s turbine blades, for instance, are exposed to hundreds of degrees of temperature as they spin at thousands of revolutions per minute. As a result, small changes are constantly taking place in the blades’ polycrystalline microstructure, but these changes cannot be empirically observed as the turbine blades turn.

“So, it is extremely important to develop predictive models that allow you to simulate the performance of this material under these high temperatures and stress so you can predict how long it will last,” says Wolf.

And, he adds, “if you want to reduce the weight of a jet engine, it would help enormously if you understood the underlying processes, so the goal of materials simulation is to put a lot more of the physics of the microstructure into [engineering] models.”

The goal of materials simulation is to increase the power-to-weight ratio by a factor of 50 to 100 percent over the next 20 years.

A “Catch-22”

The fact that most solids have crystalline structures has been known for about 100 years, but only since the mid-1990s — as a result of the development of powerful computers — have researchers had the ability to use multi-scale materials simulation to probe the secrets of the microstructures within these polycrystalline materials.

Yet the microscopic boundaries between crystals do not readily reveal their secrets. One of the quantities they pose is the “Catch-22” of materials science: to view the internal boundaries of a material would logically require cutting into the material, but once that is done, the interior surfaces become the exterior surfaces and their very nature is changed. It was to overcome such empirical limitations that researchers turned to computer simulation.

And that brought them right up against yet another seemingly insurmountable blockade. To skirt this problem the researchers devised an ingenious two-pronged approach. First, they applied a basic understanding of physics, such as Newton’s laws of motion. These same laws of motion apply to atoms as much to a large ball. And while understanding this is
A Physicist’s Best Friend

In addition to applying these basic physics concepts to the development of materials simulations, “in some very specialized cases there are experimental techniques available to statically probe the atomic structure of the interface.”

In contrast, nanocrystalline diamonds provide a case in point, since their tamarans can be probed inductively at a much higher frequency of motion than in a single atom. This distinction between Newton’s law and the viscous law of motion is important when it comes to modeling the activity of materials. Using sophisticated approaches to the microstructure, which is relevant here is to develop a fundamental understanding of materials interfaces, which gives an opportunity to simulate under physical conditions create significant wear.

Both these experiments have shown that two to three percent of all the atoms in a nanocrystalline diamond are graphite-like. And since it is known that the crystals in a diamond are pure and contain no graphite, whatever graphite shows up in the high-sensitivity experiments should be at the boundaries between the crystals. It is also known from experimental results that about five percent of all the material in a nanocrystalline diamond is in the grain boundaries.

By probing a nanocrystalline diamond with light and observing how the light is scattered, the extent to which graphite is present can be determined, and from that, other characteristics of the material can be extrapolated. “The Raman scattering gives a peek inside the diamond,” says Wolf, “but the simulations teach you a lot more than the experiments.”

Wolf, himself a physicist, and his group apply this knowledge to building models that look both at the activity within individual grain boundaries and the interaction of all the boundaries within a material. They take this approach, rather than examining what happens to all of the boundaries at the atomic level, simply because the number of atoms involved make such a task onerous. They take this approach, rather than investigating every atom, to form the boundaries of the atomic structure. This both verifies the accuracy of the simulations and gives more detailed information than the conclusions observed from the high-sensitivity experiments. This both verifies the accuracy of the simulations and gives more detailed information than the conclusions observed from the high-sensitivity experiments.

This new type of diamond material is also being tested for use as a virtually friction-free coating that holds promise for extending the life of machines in which wear creates condition for significant wear.

“Further Reading

Grain-boundary diffusion in nanocrystalline polycrystal by molecular-dynamics simulation, by D. Wolf and S. Yip, also in Physical Review B in 1997. The idea of tying a cluster together is to have a cluster supercomputer, a supercomputer that can be a supercomputer of a supercomputer of a supercomputer of a supercomputer, etc., and this is possible because of the graphite found in the grain boundaries.

Purpose of the Work

“The whole purpose of the work here is to develop a fundamental understanding of nanostructure, which is relevant to many technologies and industries. It is known from experimental results that about five percent of all the material in a nanocrystalline diamond is in the grain boundaries.”

“A SCANDINAVIAN WARRIOR

Their computer configuration is known as a Beowulf cluster, after a Scandinavian warrior whose name is the title of an Old English epic. In this case, the supercomputer is comprised of off-the-shelf personal computer components. The idea is to tie a cluster of less powerful computers together to get the power of a supercomputer.

Wolf and his colleagues opted for the Beowulf Approach for a very simple reason: money.

“Very good insulators, by turning them into conductors of electricity. These ultra-small crystal diamonds are created using vapor deposition, a process similar to that used in the manufacturing of semiconductor chips.

The idea is to choose deposition conditions such that the vapor gets deposited on an amorphous substrate, little crystallites form,” says Wolf. The result is diamonds and crystallites grown in sizes in the 5 to 10 nanometer range, which is the point where these material unique properties.

“You have steep gradients in the structure, which gives an opportunity to develop entirely new materials with properties that one never expects for these materials, and to understand those we use computer simulation, he says. It was just such simulation that showed that these diamonds are conductive because of the graphite found in their grain boundaries.

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Reversing Diamonds

Nanocrystalline diamonds also provide an example of how materials modeling is being used to help tailor specific materials to give them desirable characteristics. In this case the nanocrystalline diamond program at Argonne is reversing the characteristic of conventional diamonds, which are normally very good insulators, by turning them into conductors of electricity. These ultra-small crystal diamonds are created using vapor deposition, a process similar to that used in the manufacturing of semiconductor chips.

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In the last three years, modeling and simulation has really taken off here, basically because modeling has come of age,” says Comer. “In a lot of our projects, somebody needs results within a short period of time. Instead of weeks, we’re talking months or years. In industry, as compared to graduate school research, you have to make a conscious decision about the level of accuracy you can afford in order to deliver the results. Because even if you have the perfect results, it’s after the time when the decision had to be made, then you’ve delivered useless results.” Comer says he thrives on the mix of near-term and long-term projects that he must juggle. The more immediate projects, though not always the most technically challenging, provide what he calls “brain candy”—that quick, positive boost from seeing the tangible benefits of your work.

This means acting as a bridge to the larger modeling community and maintaining a broad network of government lab and university researchers, including key contacts made during the DOE CSGF program. His role is also to assess the research program for emerging technologies that can provide a competitive leg up, all the while keeping P&G’s trade secrets under wraps.

When they put the system in, it was pretty intimidating at first,” says Dolbow of his introduction to the corporate culture. “You’re given more than a few responsibilities right off the bat that you weren’t necessarily exposed to as a graduate student.

There is the professor’s perennial need to write research proposals for further funding, advising graduate students (he currently has two), and then developing and teaching undergraduate courses.

You have to be able to juggle all of these things simultaneously and still continue with your own research. As a PhD student you’re used to being able to devote weeks and months to a single problem and to thinking about it on a daily basis. That’s a luxury that you don’t really appreciate at the time.”

Now thriving in this multitasking role, Dolbow credits his rapid entry into academia in part to his successful graduate work with advisor Ted Belytschko, a pioneer in the engineering application of the finite element method (FEM). Belytschko’s algorithms for explicit dynamics are widely used throughout industry, in particular within the car crash simulation codes of the Big Three automakers.

One of the problems with the standard FEM, however, is that it can’t represent an arbitrary fracture path,” says Dolbow. “My PhD research was concerned with the development of more versatile methods, which are really a way of circumventing some of the inherent limitations the FEM has, principally for modeling the fracture and failure of brittle materials.”

His proposal writing efforts and research are coming together in a new National Science Foundation-sponsored project to computationally study the high-speed machining of aluminum alloys. The project is an industry-university collaboration involving researchers from Duke and Notre Dame Universities and the aluminum company Alcoa.

Thin sheets of aluminum are created by using a knife-like cutting tool to skim a layer from the top of quickly translating bulk stock. The process sometimes produces unwanted segmented chips, or fractures in the metal.

“At the outset, we’re trying to understand the fundamental failure process that occurs in the aluminum alloys at the grain scale,” says Dolbow.

In conjunction with colleague Dr. Henri Gavin, he has created WEAVE, the Web-based Educational Framework for Analysis, Visualization, and Experimentation. The online project, supported by a $540,000 NSF grant, allows engineering students to conduct lab experiments online, and from where, it suits them. (see www.nwce.duke.edu)

“Alumni Profile

Ken Comer

Procter & Gamble

while completing his phd in computational multiphase flow analysis at north carolina state university, ken comer had a lot of ideas as to the companies or government labs where he might find a job. a diaper maker wasn’t one of them.

"in the last three years, modeling and simulation has really taken off here, basically because modeling has come of age," says comer. "in a lot of our projects, somebody needs results within a short period of time. instead of weeks, we’re talking months or years. in industry, as compared to graduate school research, you have to make a conscious decision about the level of accuracy you can afford in order to deliver the results. because even if you have the perfect results, it’s after the time when the decision had to be made, then you’ve delivered useless results." comer says he thrives on the mix of near-term and long-term projects that he must juggle. the more immediate projects, though not always the most technically challenging, provide what he calls ‘brain candy’—that quick, positive boost from seeing the tangible benefits of your work.

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Marcus Martin
Sandia National Laboratories

MARCUS MARTIN IS GIVING AWAY his research. The Sandia National Labs molecular modeler wants computational and lab-based chemists to use his Monte Carlo for Complex Chemical Systems (MCCCS) program. Please:

The goal of the project is to try and get people who are interested in industry interested in using this code, and to try to get this particular code adopted by some of the academic groups. And that tends to happen a lot better if they can go in and modify the code themselves without worrying about endless licensing issues,” says Martin, a staff scientist in Sandia’s Computational Materials and Molecular Biology division.

Being a national lab researcher and code promoter means the former DOE CSGF fellow works in a realm intermediary between academic and industry researchers. He’s interested in pursuing the “big code projects” more associated with academia, but also in seeing his work applied.

The MCCCS simulation is primarily designed to understand the behavior of molecules involved in a two-phase equilibrium, an important issue in the chemical industry. The program simulates two soilless boxes, with the several hundred molecules involved being able to move between the boxes and therefore separate into vapor and liquid phases. The program was initially developed by Martin and his supervisor at the University of Minnesota, J. Ilja Siepmann, beginning in 1995.

“The chemical industry is at least interested enough that they’re using it now,” Martin says. “The prediction of vapor-liquid coexistence curves is a big deal in the chemical industry. The most common way to separate things is through distillation columns, and you need a good knowledge of the vapor-liquid coexistence to design good distillation columns.”

He’s also working with a chemical company that’s interested in applying the program to study the sorption of small molecules in polymers.

While promoting this initial application of his code, Martin is also exploring new possibilities, including its application in drug discovery and in the development of biofuels. The program is particularly useful in exploring the drug-designing problem — how a small molecule joins to a protein to inhibit its function.

“One of the things we have found is that the molecular partition between water and the active site in the protein,” Martin says. “It tends to be effective, a drug needs to preferentially absorb in the active site of the protein, yet it must also be water soluble so that it can be absorbed into the blood stream.

Martin says that extending the MCCCS Towhee program to other applications is facilitated by being part of Sandia’s critical mass of modeling with similar computational expertise that is different enough to allow for synergistic collaborations. He’s currently working with a colleague to combine the Towhee code with the Tramonto molecular theory code in order to do more efficient simulations in water.

It’s collaboration that has Martin knocking on new doors — those of biologists this time — and looking for ways to make his innovative program useful to a new community of scientists.

To download the Towhee program see: http://www.cs.sandia.gov/projects/towhee/index.html

Alumni Directory

A

Asoman Amarchalinah
Brown University
Computational Sciences
Fellowship Years: 1990-1992
Current Status: Brown University

B

Edward Barrany
University of Iowa
Engineering Mechanics
Fellowship Years: 1991-1993
Current Status: Iowa

William Barry
Carnegie Mellon University
Computational Mechanics
Fellowship Years: 1994-1996
Current Status: University of Technology, Bangkok

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

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

Dean Brederdon
University of Utah
Computer Scince
Fellowship Years: 1995-1998
Current Status: University of Utah

Paul Bunch
Pacific University
Chemical Engineering
Fellowship Years: 1994-1997
Current Status: E.I. du Pont Company

Jeffery Butera
North Carolina A&T State University
Applied Mathematics
Fellowship Years: 1993-1997
Current Status: Hampton University

C

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

Patrick Canupp
New York University
Aerospace Engineering
Fellowship Years: 1983-1995
Current Status: Paddy Enterprises

Kent Carlson
Florida State University
Mechanical Engineering
Fellowship Years: 1981-1995
Current Status: University of Iowa

Bonnie Carpenter Cozad
University of Illinois
Mechanical Engineering
Fellowship Years: 1981-1995

Edward Chao
Princeton University
Physics
Fellowship Years: 1983-1995
Current Status: Systems Engineering — GE Medical Systems

Eric Charlton
University of Michigan
Aerospace Engineering
Fellowship Years: 1983-1996
Current Status: Lockheed Martin

Michael Chioo
Massachusetts Institute of Technology
Mechanical Engineering
Fellowship Years: 1982-1996
Current Status: Teradyne

Joshua Coo
University of Illinois
Chemical Physics
Fellowship Years: 2001
Current Status: University of Illinois

Ken Conner
North Carolina State University
Mechanical Engineering
Fellowship Years: 1981-1995
Current Status: Proctor & Gamble

John Costello
University of Arizona
Applied Mathematics
Fellowship Years: 1996-2002
Current Status: University of Arizona

Nathan Crane
University of Illinois
Civil Engineering
Fellowship Years: 1995-2002
Current Status: Sandia National Laboratories — New Mexico

Stephen Cronen-Townsend
Georgia Institute of Technology
Physics
Fellowship Years: 1991-1995
Current Status: University of Massachusetts

Robert Cruise
Indiana University
Physics
Fellowship Years: 1997-2001
Current Status: Indiana University

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

D

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

Mark Di Battista
Columbia University
Applied Physics
Fellowship Years: 1982-1994

John Delboever
University of Utah
Theoretical and Applied Mechanics
Fellowship Years: 1983-1993
Current Status: Duke University

John Costello
University of Arizona
Applied Mathematics
Fellowship Years: 1996-2002
Current Status: University of Arizona

D
Q
Alessandro Quezada University of California – Berkeley Geophysics Fellowship Years: 1997-1999

R
Nathan Rau University of Illinois Civil Engineering Fellowship Years: 2000-2001
Clifton Richardson Cornell University Physics Fellowship Years: 1991-1995
John Ritter Northwestern University Materials Science Fellowship Years: 1991-1995
David Ropp University of Arizona Applied Mathematics Fellowship Years: 1995-1998 Current Status: Sandia National Laboratories — New Mexico
Robin Rosenfeld Scripps Research Institute Nurology Fellowship Years: 1996-1997 Current Status: Scripps Research Institute

S
Elsie Simpson Pierce University of Illinois Nuclear Engineering Fellowship Years: 1990-1993 Current Status: Lawrence Livermore National Laboratory


Steven Smith North Carolina State University Chemical Engineering Fellowship Years: 1993-1994 Current Status: E.I. DuPont
Rajeev Surati Massachusetts Institute of Technology Electrical Engineering Fellowship Years: 1995-1996 Current Status: Newsweb

T
Mayya Tokman California Institute of Technology Applied Mathematics Fellowship Years: 1996-2000 Current Status: University of California — Berkeley
Mario Trujillo University of Illinois Mechanical Engineering Fellowship Years: 1997-2000 Current Status: Los Alamos National Laboratory

U
Anton Van Der Ven Massachusetts Institute of Technology Materials Science Fellowship Years: 1990-2000 Current Status: 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: 1993-1995

Current Status: Electra Laboratory

W
Phillip Weeber University of North Carolina Environmental Science & Engineering Fellowship Years: 1984-1996

Adam Wellmer Princeton University Chemical Engineering Fellowship Years: 2001-2002 Current Status: Princeton University

Current Status: Scripps Research Institute

W
Philipp Weeber University of North Carolina Environmental Science & Engineering Fellowship Years: 1984-1996

Adam Wellmer Princeton University Chemical Engineering Fellowship Years: 2001-2002 Current Status: Princeton University

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

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

Z
Charles Zeeb Colorado State University Mechanical Engineering Fellowship Years: 1995-1997 Current Status: Colorado State University

For more information on DOE CSGF Alumni visit www.krellinst.org/csgf/alumni
Allison Baker
University of Colorado
Applied Mathematics
Advisor: Elizabeth Jessop
Practice: Sandia National Laboratories – New Mexico
Contact: allison.baker@colorado.edu
Research Synopsis:
My current research focuses on reducing memory access costs when solving the linear system Ax=b. A large, sparse and non-symmetric A is of interest. I am focusing on variants of the generalised minimum residual (GMRES) algorithm. I would like to gain efficiency by reducing memory access costs (primarily by increasing re-use of A) through algorithmic changes in GMRES.

Lewis Jonathan Dural
University of Chicago
Astronomy
Advisor: Robert Resner
Practice: Sandia National Laboratories – Livermore
Contact: lewis.dural@uchicago.edu
Research Synopsis:
My current research involves working on and using our center’s FLASH code to understand turbulent (thermoclar) combustion in compressible fluids. Another interesting part of my work is working on modules or algorithms which may be known in other communities, but not necessarily the astrophysical community. I’m working on a ‘Level Set’ module for the FLASH code to do flame tracking or general interface tracking; this is a very useful technique, but one which is still fairly new in these sorts of simulations.

Adrian Hill
Carnegie Mellon University
Mathematics, Algorithms & Computing
Advisor: Dennis Gabor
Practice: Sandia National Laboratories – Livermore
Contact: Adrian.hill@andrew.cmu.edu
Research Synopsis:
In the past, coarse-grain models have successfully modeled different forms of viscosity, coolant nucleation, and crack propagation. In my current work, a finite element model (FEM) with a X-par and Nekhleman surface potential implemented into the framework has been used. The X-par and Nekhleman potential, derived from molecular dynamics and applicable for modeling fracture surfaces, is rate-independent and phenomena when applied to large length scales. Current efforts are directed toward validating this model with experimental measurements from a little pipe.

Glenn Hammond
University of Illinois
Engineering & Science
Advisor: Bernd Vakakis
Practice: Los Alamos National Laboratory
Contact: ghammond@lulu.com
Research Synopsis:
I am looking at developing a method of preconditioning which better preserves parallel efficiency. Recently, researchers at Los Alamos National Laboratory developed a physics-based (operator-split) preconditioner for their radiation transport codes. I am applying this technique to the more sophisticated (more degrees of freedom per spatial node and more complex chemistry) multicomponent transport utilizing a Jacobian-free, Newton-Krylov as a smoother (PETSc) framework. This parallel transport model is built upon the PETSc library developed at Argonne National Laboratory.

Charles Hindman
University of Colorado
Aerospace Engineering
Advisor: Maria Bialas
Practice: Lawrence Livermore National Laboratory
Contact: hindman@colorado.edu
Research Synopsis:
Practicum:
Los Alamos National Laboratory – New Mexico
Research Synopsis:
The course of research undertaken under this fellowship involves applying ideas from control theory to the problem of large-scale aeroelastic system simulation. Specifically, the goal is to develop algorithms and techniques for integrating the effects of active control surfaces on an existing 200,000+ degrees of freedom aeroelastic system simulation.

Eric Lee
Argonne University
Mechanical Engineering
Advisor: Constantine Mavroidis
Practice: Sandia National Laboratories – New Mexico
Contact: ching@l39.darm.rutgers.edu
Research Synopsis:
One of the most important spatial, task oriented robotic system design problems is the Rigid Body Guidance Problem. This is the calculation of the geometric parameters of a mechanical system so that it guides a rigid body in a number of specified spatial locations. This project will focus on the development of computational design algorithms for the spatial rigid body guidance problem with serial manipulators.

Jason Hunt
University of Michigan
Aerospace Engineering & Scientific Computing
Advisor: Kenneth Powell
Practice: Lawrence Livermore National Laboratory
Contact: jhunt@engin.umich.edu
Research Synopsis:
The goal of my research is to extend current Computational Fluid Dynamic (CFD) techniques for solving mapping geometry problems to three dimensions and to incorporate current developments in Cartesian mesh generation for component-based geometry and finite-volume schemes for the Euler equations. Both turbo-machinery and helicopters, two current-motivational examples, have rotating components that are difficult to model with conventional techniques. This research will produce methods to obtain more representative simulations of flow through compressors, rotor/stator configurations (e.g., stator blades remain stationary while the rotor blades sweep through the domain), and even flow about helicopters.

Diem-Phuong Nguyen
University of Utah
Chemical Engineering
Advisor: Philip Smith
Practice: Lawrence Livermore National Laboratory
Contact: duenhan@llnl.gov
Research Synopsis:
In the area of numerical simulation of accidental fires and explosions, there is no computational fluid dynamics (CFD) code available that calculates both turbulent reacting flows and complex chemical kinetics. Due to limitations of computational time and space, existing CFD codes available are codes which model only laminar flows and complex chemistry or turbulent flows and no chemistry or simple one-step chemistry. The most innovative aspect of my research is that through introduction of a subgrid scale (SGS) reaction model, practical reacting flow may be accurately simulated. SGS models perform calculations which allow for simulation of practical reacting flow situations by bridging microscopic details to macroscopic domain.

Christopher Oehmen
University of Memphis
Biomedical Engineering
Advisor: Samath Denu
Practice: Lawrence Livermore National Laboratory
Contact: coehmen@memphis.edu
Research Synopsis:
My research deals with the modeling of highly nonlinear biological systems. Specifically, my aim is to create 2D and 3D models of pacing cardiac cell networks which take into account electrical activity of the cell membranes, as well as the electrical effects from diffusion and electric fields acting on ionic in the tissue. My hypotheses are that (i) diffusion, which is conventionally considered trivial, is a crucial element of entrainment and propagation in the spatial node (SAN), or the origin of pacing, and (ii) incorporation of geometric information into the diffusion and electric field calculations for electrical activity in the SAN will improve the ability of tissue level models to explain the experimentally observed effects of drugs and pathophysiologival conditions on propagation in the SAN.

Notable:
Invited to and attended the 2001 Noble Laureate Conference in Llandudno, Germany.
**FIRST YEAR FELLOWS**

Bree Aldridge  
Massachusetts Institute of Technology  
Computational Biology  
Advisor: Douglas Lauffenburger  
Contact: breea@mit.edu

Teresa Bailey  
Texas A&M University  
Engineering  
Advisor: Marvin Adams  
Contact: baileyte@tamu.edu

Michael Barad  
University of California – Davis  
Environmental Modelling  
Advisor: Geoffrey Schulz  
Contact: mbarad@ucdavis.edu

Jaydeep Bardhan  
Massachusetts Institute of Technology  
Electrical Engineering  
Advisor: Jacob White  
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Kevin Chu  
Massachusetts Institute of Technology  
Applied Mathematics  
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Owen Hofmeyer  
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Carnegie Mellon University  
Computational Neuroscience  
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Contact: oben@princeton.edu

Joshua Waterfall  
Cornell University  
Biophysics  
Advisor: James Sethna  
Contact: jalex@cornell.edu

Michael Wu  
University of California – Berkeley  
Computational Neuroscience  
Advisor: Jack Gallant  
Contact: wafting@uclink4.berkeley.edu