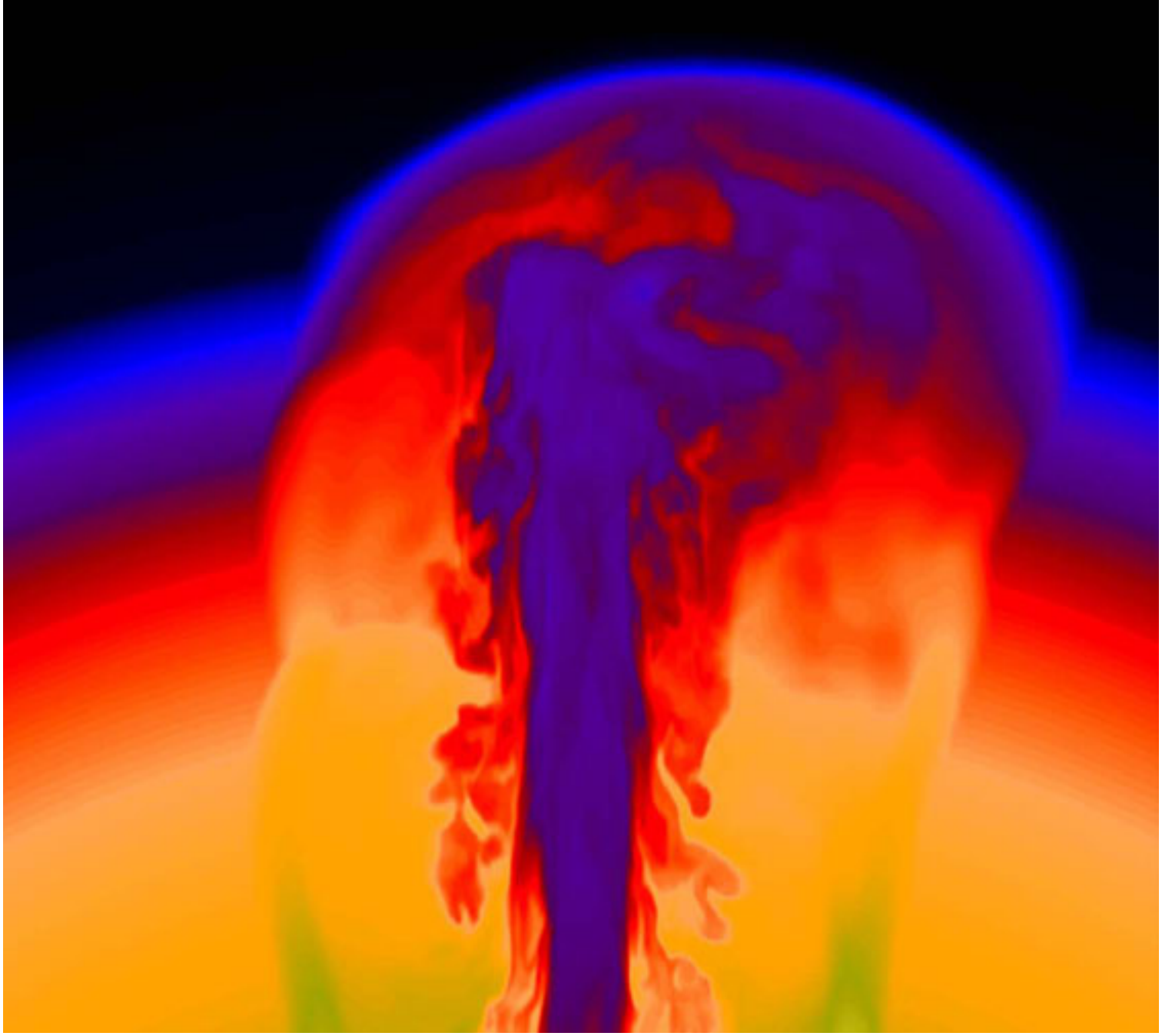
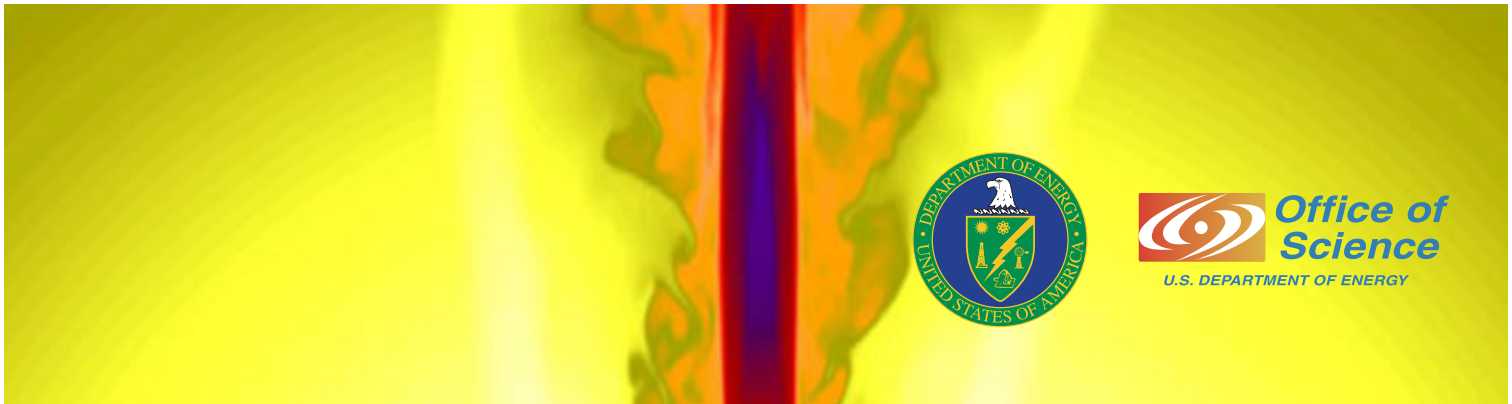


SCIENTIFIC DISCOVERY

A progress report on the U.S. Department of Energy's Scientific Discovery through Advanced Computing Program



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Cover: When the cores of massive stars collapse to form black holes and accretion disks, relativistic jets known as gamma ray bursts pass through and then explode the star. SciDAC's Supernova Science Center used simulations like the one of the cover to test and confirm theories about the origin of gamma-ray bursts.

SCIENTIFIC DISCOVERY

A progress report on the U.S. Department of Energy's Scientific Discovery through Advanced Computing Program

Office of Science
U.S. DEPARTMENT OF ENERGY

SciDAC
Scientific Discovery through Advanced Computing

Executive Summary

Greetings:

Five years ago, the U.S. Department of Energy Office of Science launched an innovative software development program with a straightforward name – Scientific Discovery through Advanced Computing, or SciDAC. The goal was to develop scientific applications to effectively take advantage of the terascale supercomputers (capable of performing trillions of calculations per second) then becoming widely available.

From the most massive explosions in our universe to our planet's changing climate, from developing future energy sources to understanding the behavior of the tiniest particle, the SciDAC program has lived up to its name by helping scientists make important discoveries in many scientific areas.

Here are some examples of the achievements resulting from SciDAC:

- For the first time, astrophysicists created fully resolved simulations of the turbulent nuclear combustion in Type 1a supernovae, exploding stars which are critical to better understanding the nature of our universe.
- Using climate modeling tools developed and improved under SciDAC, climate change scientists in the United States are making the largest contribution of global climate modeling data to the world's leading body on climate studies, the Intergovernmental Panel on Climate Change.
- To better understand combustion, which provides 80 percent of the energy used in the United States, scientists created the first laboratory-scale flame simulation in three dimensions, an achievement which will likely help improve efficiency and reduce pollution.
- Looking toward future energy resources, magnetic fusion researchers, applied mathematicians and computer scientists have worked together to successfully carry out advanced simulations on the most powerful modern supercomputing platforms. They discovered the favorable result that for the larger reactor-scale plasmas of the future such as ITER (the planned international fusion experiment), heat losses caused by plasma turbulence do not continue to follow the empirical trand of increasing with the size of the system.
- To make the most of existing particle accelerators and reduce the cost of building future accelerators, teams developed new methods for simulating improvements. In addition to helping us understand the most basic building blocks of matter, accelerators make possible nuclear medicine.
- Physicists studying the Standard Model of particle interactions have, after 30 years of trying, been able to model the full spectrum of particles known as hadrons at the highest level of accuracy ever. The results could help lead to a deeper understanding of the fundamental laws of physics.

These and other impressive scientific breakthroughs are the results of hundreds of researchers working in multidisciplinary teams at national laboratories and universities across the country.

The SciDAC Program consisted of three research components:

- Creating a new generation of scientific simulation codes to take full advantage of the powerful computing capabilities of terascale supercomputers
- Creating the mathematical and computing systems software to enable these scientific simulation codes to effectively and efficiently use terascale computers
- Creating a distributed science software infrastructure to enable scientists to effectively collaborate in managing, disseminating and analyzing large datasets from large-scale computer simulations and scientific experiments and observations.

Not only did the researchers work in teams to complete their objectives, but the teams also collaborated with one another to help each other succeed. In addition to advancing the overall field of scientific computing by developing applications which can be used by other researchers, these teams of experts have set the stage for even more accomplishments.

This report will describe many of the successes of the first five years of SciDAC, but the full story is probably too extensive to capture – many of the projects have already spurred researchers in related fields to use the applications and methods developed under SciDAC to accelerate their own research, triggering even more breakthroughs.

While SciDAC may have started out as a specific program, Scientific Discovery through Advanced Computing has become a powerful concept for addressing some of the biggest challenges facing our nation and our world.

Michael Strayer

SciDAC Program Director
U.S. Department of Energy
Office of Science

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Scientific Discovery through Advanced Computing

Over the past 50 years, computers have transformed nearly every aspect of our lives, from entertainment to education, medicine to manufacturing, research to recreation. Many of these innovations are made possible by relentless efforts by scientists and engineers to improve the capabilities of high performance computers, then develop computational tools to take full advantage of those capabilities.

As these computer systems become larger and more powerful, they allow researchers to create more detailed models and simulations, enabling the design of more complex products, ranging from specialized medicines to fuel-efficient airplanes. Critical to the success of these efforts is an every-increasing understanding of the complex scientific processes and principles in areas such as physics, chemistry and biology.

Over the past five years, teams of scientists and engineers at national laboratories operated by the U.S. Department of Energy, along with researchers at universities around the country, have been part of a concerted program to accelerate both the performance of high performance computers and the computing allocations used to advance our scientific knowledge in areas of critical importance to the nation and the world.

Launched in 2001, this broad-based program is called Scientific Discovery through Advanced Computing, or SciDAC for short. The $57 million-per-year program was designed to accelerate the development of a new generation of tools and technologies for scientific computing. SciDAC projects were selected to capitalize on the proven success of multidisciplinary scientific teams. In all, 51 projects were announced involving collaborations among 13 DOE national laboratories and more than 50 colleges and universities.

SciDAC is an integrated program that has created a new generation of scientific simulation codes. The codes are being created to take full advantage of the extraordinary computing capabilities of today's terascale computers (computers capable of doing trillions of calculations per second) to address ever larger, more complex problems. The program also includes research on improved mathematical and computing systems software that will allow these codes to use modern parallel computers effectively and efficiently. Additionally, the program is developing "collaboratory" software to enable geographically separated scientists to effectively work together as a team, to control scientific instruments remotely and to share data more readily.

Today, almost five years after it was announced, the SciDAC program has lived up to its name and goal of advancing scientific discovery through advanced computing.

Teaming Up for Better Science

In the 1930s, physicist Ernest Orlando Lawrence pioneered a new approach to scientific research. Rather than working alone in their labs, physicists, engineers, chemists and other scientists were brought together to form multidisciplinary teams which could bring a range of knowledge and expertise to bear on solving scientific challenges. This "big science" approach formed the basis for the national laboratories operated by the Department of Energy.

Since the 1950s, scientists at the DOE national labs have increasingly employed high performance computers in their research. As a result, computational science has joined experimental science and theoretical science as one of the key methods of scientific discovery.

With SciDAC, this approach has come full circle, with mutlidisciplinary teams from various research institutions working together to develop new methods for scientific discovery, while also developing technologies to advance collaborative science.

And as with other research accomplishments, the results are being shared through articles published in scientific and technical journals. Additionally, the tools and techniques developed under the SciDAC program are freely available to other scientists working on similar challenges.

A Full Spectrum of Scientific Discovery

The SciDAC program was created to advance scientific research in all mission areas of the Department of Energy's Office of Science. From looking back into the origins of our

universe to predicting global climate change, from researching how to burn fuels more efficiently and cleanly to developing environmentally and economically sustainable energy sources, from investigating the behavior of the smallest particles to learning how to combine atoms to create new nanotechnologies, computational science advanced under SciDAC affects our lives on many levels.

Today, almost five years after it was announced, the SciDAC program has lived up to its name and goal of advancing scientific discovery through advanced computing. This progress report highlights a number of the scientific achievements made possible by SciDAC and also looks at the computing methods and infrastructure created under the program which are now driving computational science advances at research institutions around the world.

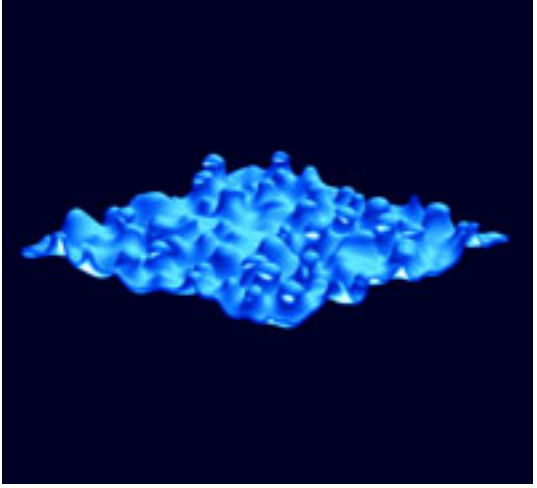
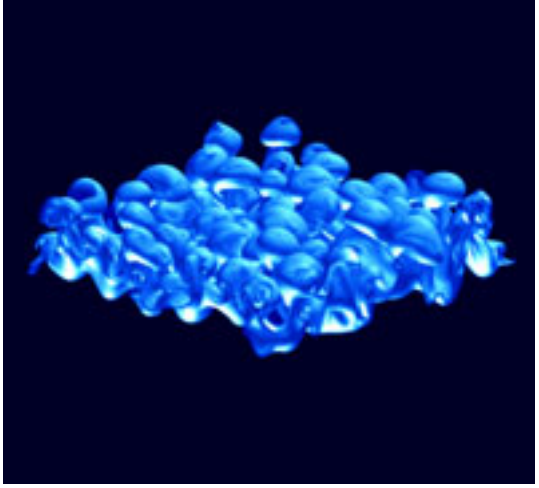
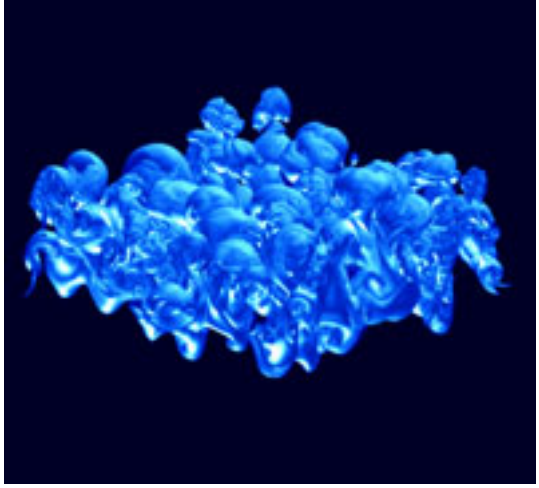
The achievements range from understanding massive exploding stars known as supernovae to studying the tiniest particles which combine to form all the matter in the universe. Other major accomplishments include better methods for studying global climate, developing new sources of energy, improving combustion to reduce pollution and designing future facilities for scientific research.

Computing then and now

While the achievements of the SciDAC teams are impressive on their own, they also demonstrate just how far scientific computing has come in the past 20 years.

Back in 1986, a state-of-the-art supercomputer was a Cray-2, which had a peak speed of 2 gigaflops (2 billion calculations) per second and a then-phenomenal 2 gigabytes of memory. Such machines were rare, located only at a limited number of research institutions, and access was strictly controlled. Scientific programs were typically written by individuals, who coded everything from scratch. Tuning the code to improve performance was done by hand – there were no tools freely available, no means of creating visualizations. The lucky scientists were able to submit jobs remotely using a 9600 baud modem.

Today, inexpensive highly parallel commodity clusters provide teraflops-level performance (trillions of calculations per second) and run on open source software. Extensive libraries of tools for high performance scientific computing are widely available – and expanding, thanks to SciDAC. Computing grids offer remote access at 10 gigabits per second, allowing hundreds or thousands of researchers to use a single supercomputer. Scientists can do code development on desktop computers which have processors faster than the Cray-2 and offer more memory. Once an application runs, powerful visualization tools provide detailed images which can be manipulated, studied and compared to experimental results.

Supernovae Science:

Earth-Based Combustion Simulation Tools Yield Insights into Supernovae

In the far reaches of space, a small star about the size of Earth simmers away, building up the heat and pressure necessary to trigger a massive thermonuclear explosion.

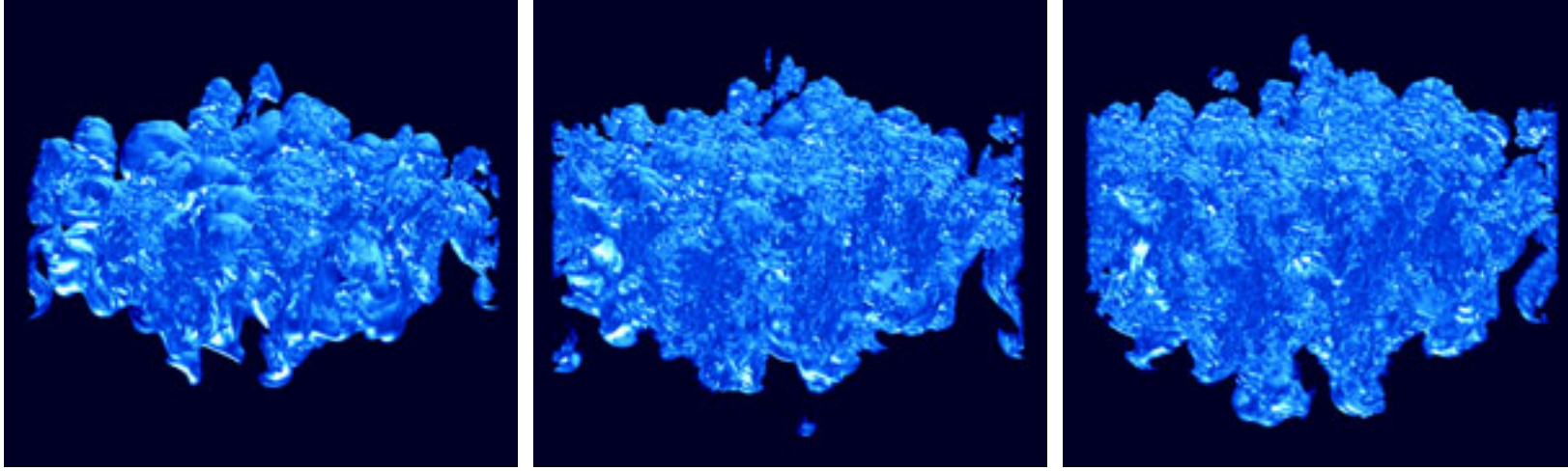


FIGURE 1. This series shows the development of a Rayleigh-Taylor unstable flame. The interface between the fuel and ash is visualized The buoyant ash rises upward as the fuel falls downward in the strong gravitational field, wrinkling the flame front. This increases the surface area of the flame and accelerates the burning. At late times, the flame has become fully turbulent.

The star, known as a white dwarf, consists of oxygen and carbon. At its center, the star is about two billion times denser than water. Already 40 percent more massive than our Sun, the star continues to gain mass as a companion star dumps material onto the surface of the white dwarf.

As this weight is added, the interior of the star compresses, further heating the star. This causes the carbon nuclei to fuse together, creating heavier nuclei. The heating process, much like a pot of water simmering on the stove, continues for more than 100 years, with plumes of hot material moving through the star by convection and distributing the energy.

Eventually, the nuclear burning occurs at such a rate that convection cannot carry away all the energy that is generated and the heat builds dramatically. At this point, a burning thermonuclear flame front moves quickly out from the core of the star, burning all the fuel in a matter of seconds. The result is a Type Ia supernova, an exploding star which is one of the brightest objects in the universe. Because of their brightness, supernovae are of great interest to astrophysicists studying the origin, age and size of our universe.

Although astronomers have been observing and recording supernovae for more than 1,000 years, they still don't understand the exact mechanisms which cause a white dwarf to explode as a supernova. Under SciDAC, teams of researchers worked to develop computational simulations to try to understand the processes. It turns out that an algorithm developed to simulate a flame from a Bunsen burner in a laboratory is well suited – with some adaptation – to studying the flame front moving through a white dwarf.

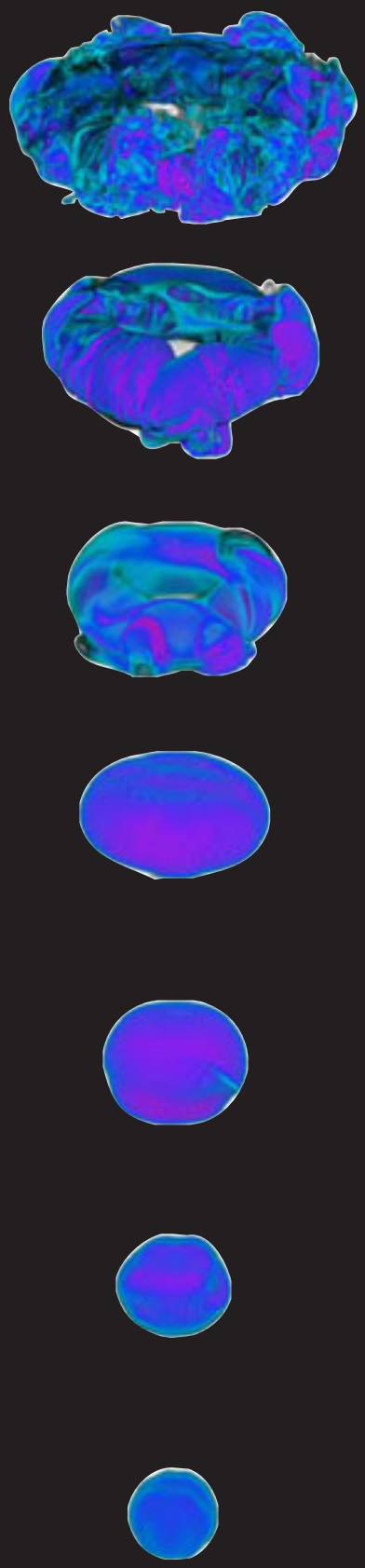
The SciDAC program brought together members of the Supernova Science Center project and LBNL mathematicians and computational scientists associated with the Applied Partial Differential Equations Integrated Software Infrastructure Center (ISIC). "We had two groups in very different fields," said Michael Zingale, a professor at the State University of New York–Stony Brook and member of the Supernovae Science Center. "We met with these mathematicians who had developed codes to study combustion and through SciDAC, we started using their tools to study astrophysics."

The adaptive mesh refinement (AMR) combustion codes developed at the Center for Computational Sciences and Engineering (CCSE) at Lawrence Berkeley National Laboratory are very effective for modeling slow-moving burning fronts. The behavior of the flame front leading up to a supernova is very similar, and the scientists worked together to adapt the codes to astrophysical environments.

Computational scientists tackle such problems by dividing them into small cells, each with different values for density, pressure, velocity and other conditions. The conditions are then evolved one time step at a time, using equations which say how things like mass, momentum and energy change over time, until a final time is reached. The astrophysicists had been using a code that included modeling the effects of sound waves on the flame front, which limited them to very small time steps. So, modeling a problem over a long period of time exceeded the availability of computing resources. The CCSE code allowed the astrophysicists to filter out the sound waves, which aren't important in this case, and take much bigger time steps, making more efficient use of their supercomputing allocations.

The net result, according to Zingale, is that the project team was able to carry out studies which had never been possible before. Their findings have been reported in a series of papers published in scientific journals such as Astrophysical Journal.

While observational astronomers are familiar with the massive explosion which characterizes a Type Ia supernova, one of the unknowns is where the flame starts, or if it starts in more than one location. When the



flame front starts out, it is moving at about one one-thousandth of the speed of sound. As it burns more fuel, the flame front speeds up. By the time the star explodes, the front must be moving at half the speed of sound. The trick is, how does it accelerate to that speed?

One answer explored by the SciDAC team is the effect of a wrinkled flame. As the flame becomes wrinkled, it has more surface area, which means it burns more fuel, which in turn accelerates the flame front. The AMR codes were used to model small areas of the flame front in very high resolution.

As the flame burns, it leaves in its wake "ash," which through intense heat and pressure is fused into nickel. This hot ash – measuring several billion degrees Kelvin – is less dense than the fuel. The fuel ahead of the front is relatively cooler, at about 100 million degrees Kelvin, and denser than the ash. These conditions make the flame front unstable. This instability, known as the Rayleigh-Taylor instability, causes the flame to wrinkle.

As the flame starts out from the center and burns through most of the star, the front between the fuel and the ash is sharp and the front is called a "flamelet."

Astrophysicists had predicted that as the flame front burns further out from the center, the lower density of the star would cause it to burn less vigorously and become more unstable due to increased turbulence and mixing of fuel and ash. This represents a different mode of combustion known as a "distributed burning regime." Scientists believe that such combustion occurs in the late stage of a supernova explosion.

Using the AMR combustion codes and running simulations for 300,000 processor hours at DOE's National Energy Research Scientific Computing Center, the Supernova Science Center team was able to create the first-ever three-dimensional simulations of such an event. The results are feeding into the astrophysics community's knowledge base.

"While other astrophysicists are modeling entire stars at a different scale, they need to know what is going on at scales their models can't resolve – and we're providing that model for them," Zingale said. "Although it takes a large amount of computing time, it is possible now thanks to these codes. Before our SciDAC partnership, it was impossible."

FIGURE 2. This series of images show the growth of a buoyant reactive bubble. At the density simulated, the rise velocity is greater than the laminar flame velocity, and the bubble distorts significantly. The vortical motions transform it into a torus. Calculations of reactive rising bubbles can be used to gain more insight into the early stages of flame propagation in Type Ia supernovae.

From Soundwaves to Supernova:

SciDAC Provides Time, Resources to Help Astrophysicists Simulate a New Model

Once every 30 to 50 years – and then just for a few milliseconds – an exploding star known as a core-collapse supernova is the brightest object in the universe, brighter than the optical light of all other stars combined.

Supernovae have been documented for 1,000 years and astrophysicists know a lot about how they form, what happens during the explosion and what's left afterward. But for the past 40 years, one problem has dogged astrophysicists – what is the mechanism that actually triggers the massive explosion? Under SciDAC, a number of computational projects were established to simulate plausible explanations. One group created simulations showing a new mechanism for core-collapse supernovae. This model indicates that the core of the star generates sound waves which in turn become shock waves powerful enough to trigger the explosion.

Understanding these explosions and their signals is important, not only because of their central role in astronomy and nucleosynthesis, but because a full understanding of supernovae may lead to a better understanding of basic physics.

The massive stars which become supernovae feature a number of conditions which are also found on Earth – winds, fluid flows, heating and cooling. But whereas a hurricane may blast along at 150 kilometers an hour on earth, the winds on these stars rage at tens of kilometers per second. The temperature of the star is 100 million times that of Earth, and the density of the object can be 14 orders of magnitude more dense than lead.

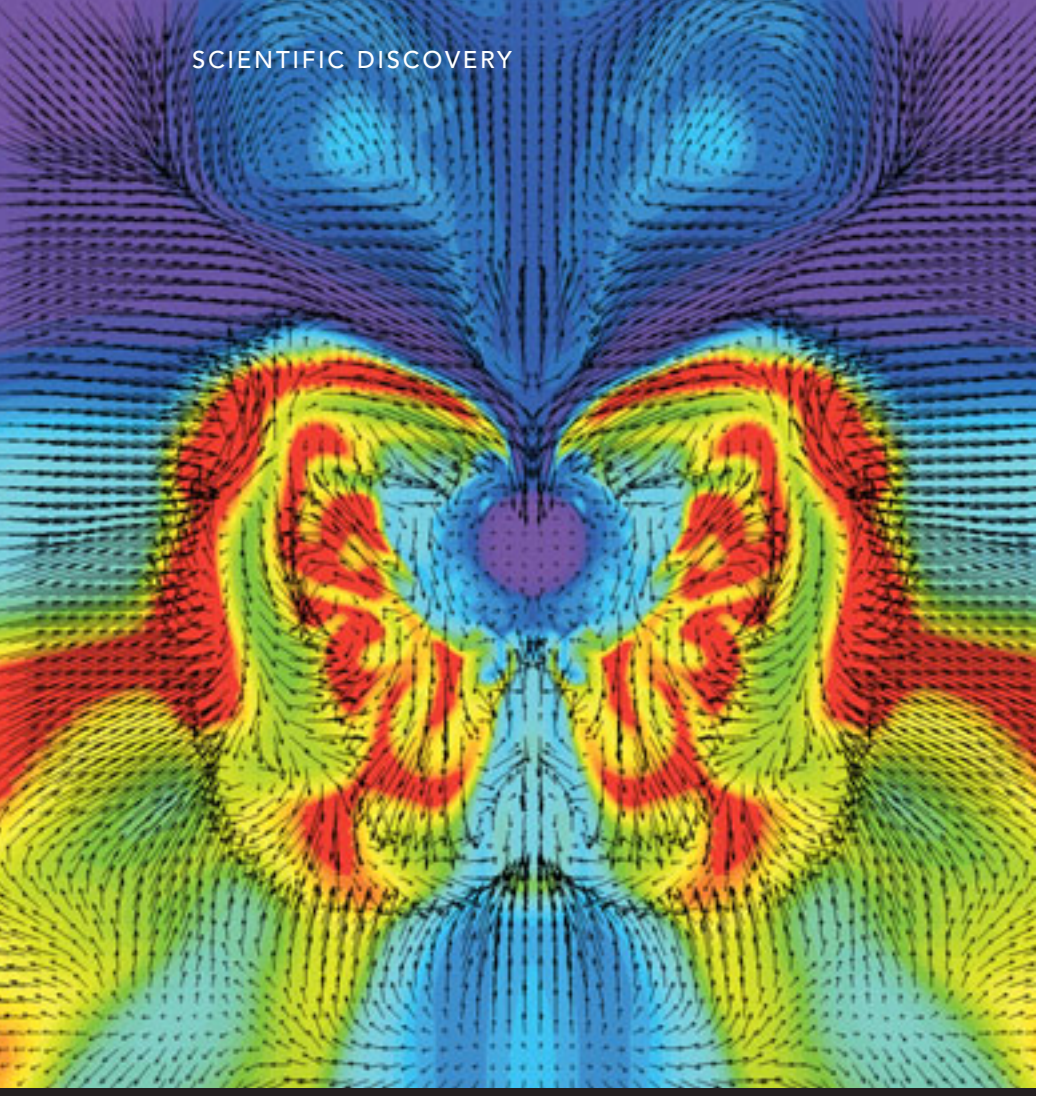
In short, studying supernovae is a very complicated problem. Key to finding an answer is understanding the physics of all the interactions in the star.

One thing that is known is that supernovae produce neutrinos, particles with very little mass which travel through space and everything in their path. Neutrinos carry energy from the deep interior of the star, which is being shaken around like a jar of supersonic salad dressing, and deposit the energy on the outer region. One theory holds that if the neutrinos deposit enough energy throughout the star, this may trigger the explosion.

To study this, a group led by Adam Burrows, professor of astronomy at the University of Arizona and a member of the SciDAC Supernova Science Center, developed codes for simulating the behavior of a supernovae core in two dimensions. While a 3D version of the code would be optimum, it would take at least five more years to develop and would require up to 300 times as much computing time. As it was, the group ran 1.5 million hours of calculations at DOE's National Energy Research Scientific Computing Center.

But the two-dimensional model is suitable for Burrows' work, and the instabilities his group is interested in studying can be seen in 2D. What they found was that there is a big overturning motion in the core, which leads to wobbling, which in turn creates sound waves. These waves then carry energy away from the core, depositing it farther out near the mantle.

According to Burrows, these oscillations could provide the "power



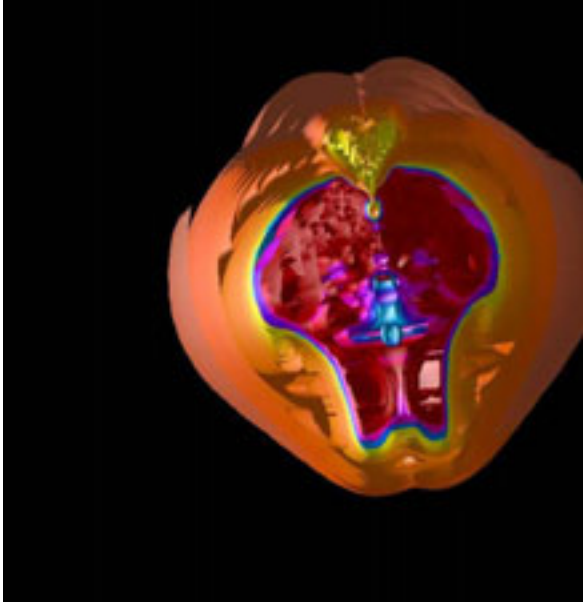


FIGURE 3. A 2D rendition of the entropy field of the early blast in the inner 500 km of an exploding supernova. Velocity vectors depict the direction and magnitude of the local flow. The bunching of the arrows indicates the crests of the sound waves that are escalating into shock waves. These waves are propagating outward, carrying energy from the core to the mantle and helping it to explode. The purple dot is the protoneutron star, and the purple streams crashing in on it are the accretion funnels. (All images courtesy of Adam Burrows, University of Arizona)

source" which puts the star over the edge and causes it to explode. To imagine what such a scenario would look like, think of a pond into which rocks are thrown, causing waves to ripple out. Now think of the pond as a sphere, with the waves moving throughout the sphere. As the waves move from the denser core to the less dense mantle, they speed up. According to the model, they begin to crack like a bullwhip, which creates shockwaves. It is these shockwaves, Burrows believes, which could trigger the explosion.

So, what led the team to this model? They came up with the idea by following the pulsar – the neutron star which is the remains of a supernova. They wanted to explore the origin of the high speed which pulsars seem to be born with and this led them to create a code that allowed the core to move. However, when they implemented this code, the core not only recoiled, but oscillated, and generated sound waves.

The possible explosive effect of the oscillations had not been considered before because previous simulations of the conditions inside the core used smaller time steps, which consumed more computing resources. With this limitation, the simulation ran their course before the onset of oscillations. With SciDAC support, however, Burrows' team was able to develop new codes with larger time steps, allowing them to model the oscillations for the first time.

Calling the simulation a "real

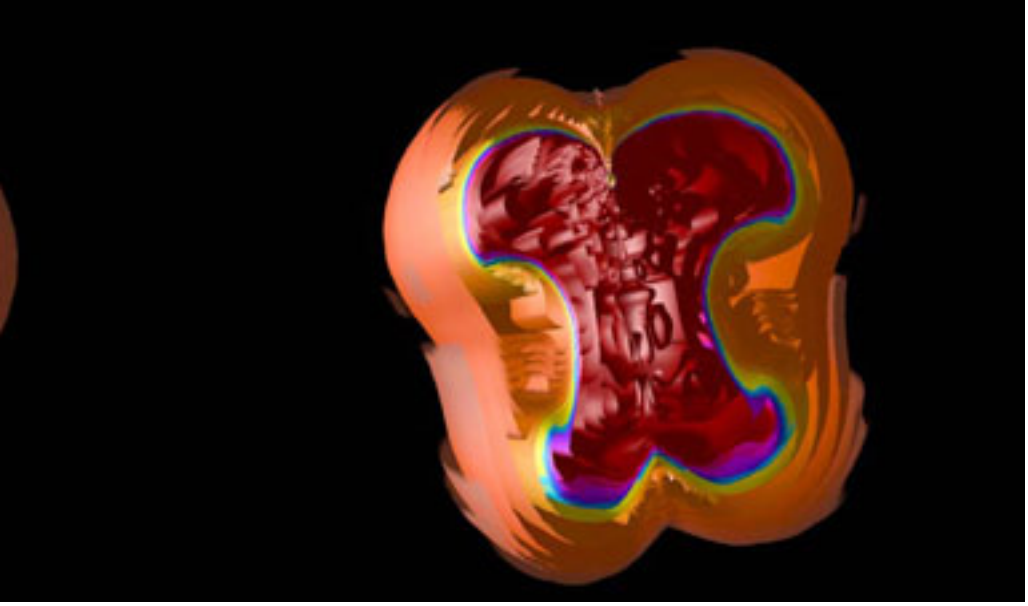


FIGURE 4. These shells are isodensity contours, colored according to entropy values. The red (blast area) indicates regions of high entropy, and the orange outer regions have low entropy. In the image on the left, matter is accreting from the top onto the protoneutron star in the center (the orange dot that looks like the uvula in the throat). The image is oriented so that the anisotropic explosion is emerging down and towards the viewer. The scale is roughly 5000 km. The image on the right shows the same explosion later in time and at a different orientation with respect to the viewer.

numerical challenge," Burrows said the resulting approach "liberated the inner core to allow it to execute its natural multidimensional motion." This motion led to the excitation of the core, causing the oscillations at a distinct frequency.

SciDAC made the work possible, he said, by providing support over five years – enough time to develop and test the code – and the computing resources to run the simulations. The results look promising, but as is often the case, more research is needed before a definitive mechanism for triggering a supernova is determined.

The group published a paper on their research in the Astrophysical Journal. Neutrino transfer is included as a central theme in a 2D multi-group, multi-neutrino, flux-limited transport scheme. It is approximate but has the important components, and is the only truly 2D neutrino code with results published in the archival literature.

"The problem isn't solved," Burrows said. "In fact, it's just beginning."

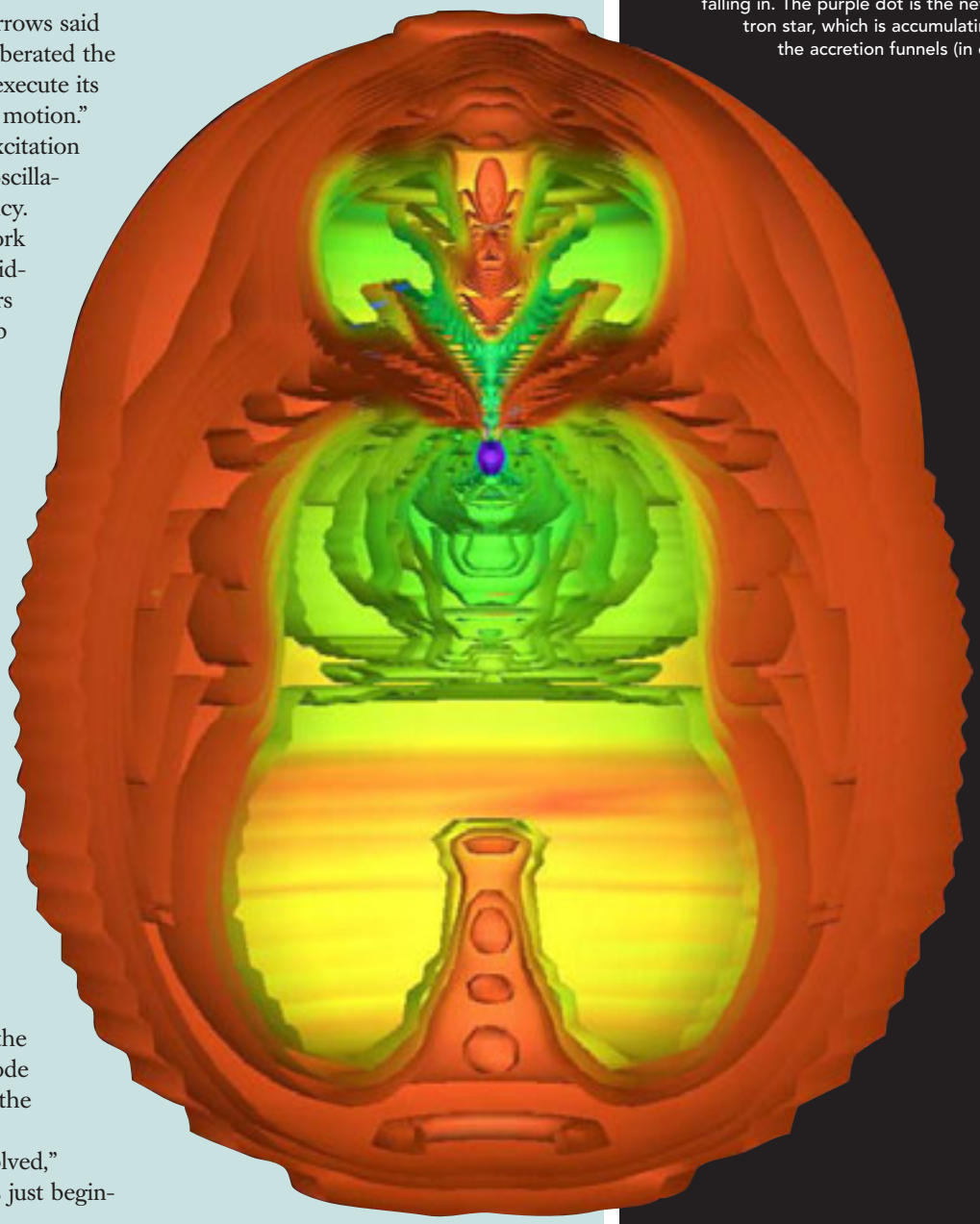


FIGURE 5. Another isodensity shell colored with entropy, showing simultaneous accretion on the top and explosion on the bottom. The inner green region is the blast, and the outer orange region is the unshocked material that is falling in. The purple dot is the newly formed neutron star, which is accumulating mass through the accretion funnels (in orange).

Insight into Supernovae:

SciDAC's Terascale Supernova Initiative Discovers New Models for Stellar Explosions, Spinning Pulsars

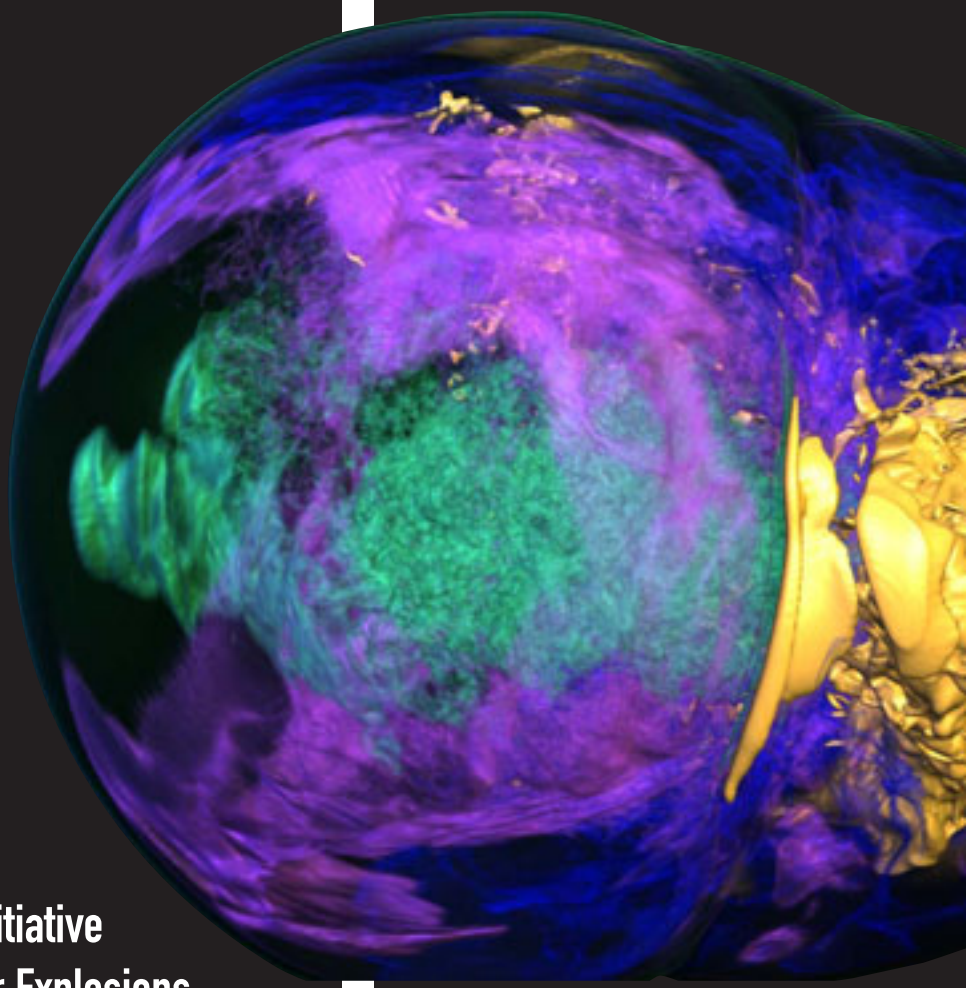
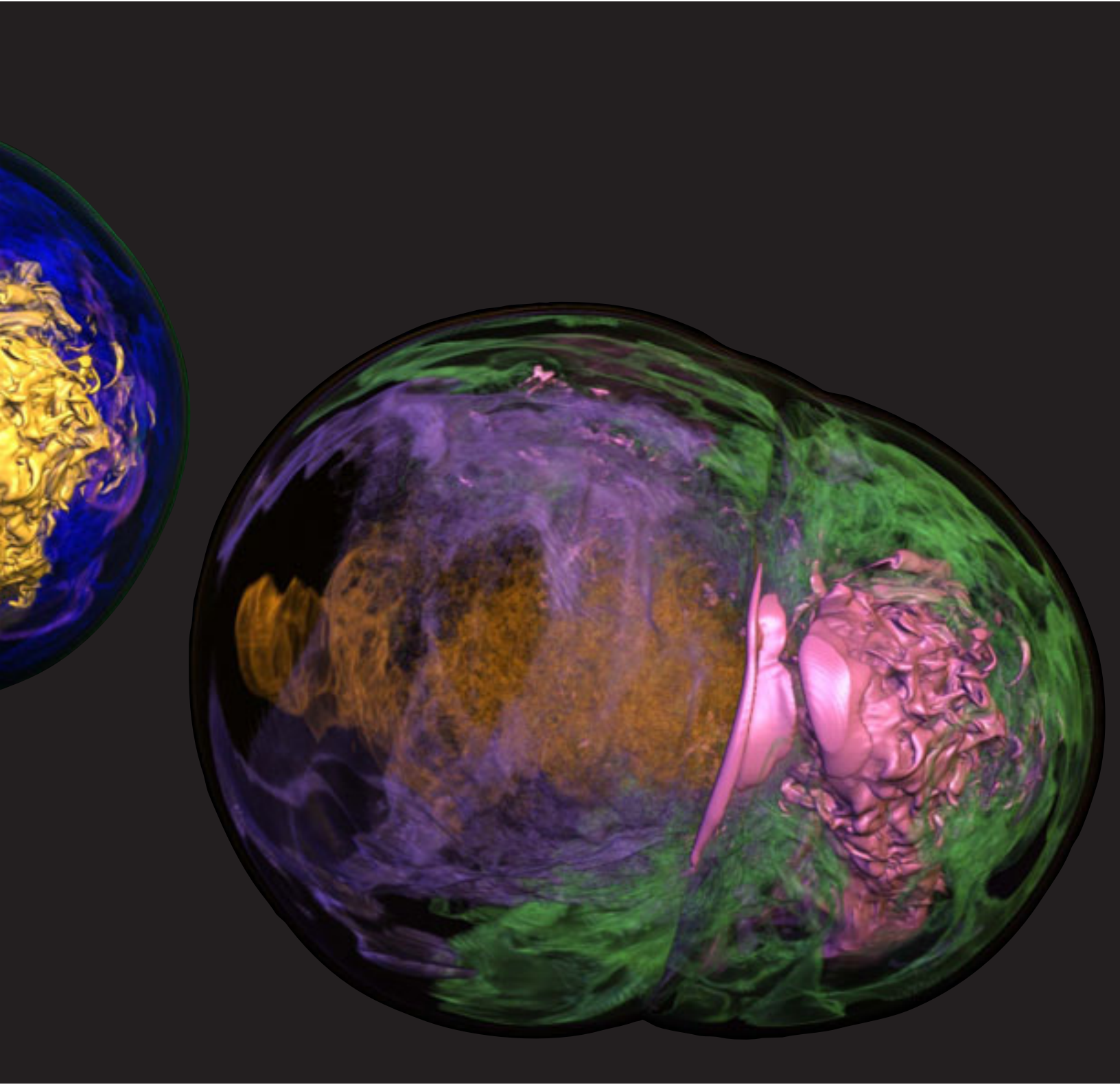


FIGURE 1: This image provides a snapshot of the angular momentum of the layered fluid flow in the stellar core below the supernova shock wave (the outer surface) during a core collapse supernova explosion. Pink depicts a significant flow rotating in one direction directly below the shock wave. Gold depicts a deeper flow directly above the proto-neutron star surface, moving in the opposite direction. The supernova shock wave instability (SASI) leads to such counter rotating flows and is important in powering the supernova, and may be responsible for the spin of pulsars (rotating neutron stars). The inner flow (in green) spins up the proto-neutron star. These three-dimensional simulations were performed by John Blondin (NCSU) under the auspices of the Terascale Supernova Initiative, led by Tony Mezzacappa (ORNL). The visualization was performed by Kwan-Liu Ma (University of California, Davis).

The massive stellar explosions known as core-collapse supernovae are not only some of the brightest and most powerful phenomena in the universe, but are also the source of many of the elements which make up our universe – from the iron in our blood cells to the planet we live on to the solar systems visible in the night sky.

Supernova science has advanced dramatically with the advent of powerful telescopes and other instruments for observing and measuring the deaths of these stars, which are 10 times more massive than our sun, or more. At the same time, increasingly accurate applications for simulating supernovae have been developed to



take advantage of the growing power of bigger and faster supercomputers.

Scientists now know that these massive stars are layered like onions. Around the iron core are layer after layer of lighter elements. As the stellar core becomes more massive, gravity causes the core to collapse to a certain point at which it rebounds like a compressed ball. This results in a shock wave which propagates from the core to the outermost layers, causing the star to explode.

Despite these gains in understanding, however, a key question remains unanswered: What triggers the forces which lead a star to explode? Under SciDAC, the Terascale Supernova Initiative (TSI) was launched, consisting of astrophysicists, nuclear physicists, computer scientists, mathematicians and networking engineers at national laboratories and universities around the country. Their singular focus was to understand how these massive stars die.

"When these stars die in stellar

explosions known as core-collapse supernovae, they produce many of the elements in the universe. In fact, they are arguably the single most important source of elements," said Tony Mezzacappa, an astrophysicist at Oak Ridge National Laboratory and principal investigator for the TSI. "Learning what triggers supernovae is tantamount to understanding how we came to be in the universe."

Ascertaining the explosion mechanism is one of the most important questions in physics. It is a complex, multi-physics problem involving fluid flow, instability, and turbulence, stellar rotation, nuclear physics, particle physics, radiation transport and magnetic fields.

"Much of modern physics comes to play a role in a core-collapse supernova," Mezzacappa says. "The cosmos is very much a physics laboratory."

Once the explosion mechanism is accurately predicted, scientists will be able to predict all the other associated byproducts and phenomena, such as the synthesis of elements. The key to solving this question depends on developing more detailed computer models, such as those advanced under SciDAC, and detailed observations of core-collapse supernovae, which only occur about twice every century in our galaxy (although many such supernovae are observed each year from outside of our galaxy). As models are developed and improved, their accuracy can be tested by comparing the results with the observed data. By adjusting any parameters of the model (of course, the goal in developing sophisticated models is to minimize the number of free parameters), scientists can generate results which are closer and closer to the actual data.

Because the simulations are computationally intensive, Mezzacappa and John Blondin, a professor at North Carolina State University, started by developing codes to look at the fluid flow at the core of a supernova. To focus on this one area, they removed the other physics components from their code, knowing they would have to add them again later. They were interested in learning how the core flow behaves during the explosion as one goes from two spatial dimensions to three. They first ran the code in two dimensions, then in 3D. When they ran the simulations, they started to see instability in the shock wave. But, Mezzacappa said, they initially believed that the physics in their code should not have led to that behavior. Their first reaction was that the code contained an error, but further study led them into a new area of supernova research.

Despite decades of supernova theory focused on the formation and propagation of the shock wave, apparently no one considered whether the shock wave was stable, according to Mezzacappa. The TSI team's research led them to conclude that the shock wave is unstable; and if it is perturbed, it grows in an unbounded, nonlinear fashion. As it spreads, it becomes more and more distorted. The TSI group found that the instability of the shock wave could help contribute to the explosion mechanism. For example, a distorted shock wave could explain why supernovae explode asymmetrically.

Under further study, the TSI researchers found that as they added more physics back into their code, the instability did not go away, giving them more confidence in their findings. Calling this new discovery the Stationary Accretion Shock Instability, or SASI, the team published their findings, which were then corroborated by other supernova researchers. As a result, Mezzacappa said, the work has fundamentally changed scientists' thinking about the explosion phenomenon. And, he adds, it probably would not have happened without the multidisciplinary approach fostered by SciDAC.

For starters, SciDAC provided the team with access to some of the world's fastest supercomputers – a resource otherwise unavailable to researchers like Blondin. This access to the Cray X1E and Cray XT3 systems at Oak Ridge gave Blondin the computing horsepower he needed to run his simulations in 3D.

But scaling up from two to three dimensions is not just a matter of running on a larger computer. It is also a matter of developing more detailed codes.

In this case, neutrinos are central to the dynamics of core-collapse supernovae. The explosion releases 10^{53} ergs of radiation, almost all of it in the form of neutrinos. The explosion energy (the kinetic energy of the ejected material) is only 10^{51} ergs. This intense emission of radiation plays a key role in powering the supernova, heating the interior material below the shock wave and adding energy to drive the shock wave outward. But this radiation transport – the production, movement and interaction of the neutrinos – is one of the most difficult things to simulate computationally. It requires that the supercomputer solve a huge number of algebraic equations. Applied mathematicians on the TSI team developed methods for solving the equations on terascale supercomputers.

"This is another example of how SciDAC makes a world of difference – we could not have done these simulations without the help of the applied mathematicians," Mezzacappa said. "SciDAC really enabled us to think about this problem in all of its complexity in earnest for the first time."

But this also led to a new challenge. Suddenly, the team was faced with managing massive amounts of data with no infrastructure for analyzing or visualizing these terabytes of data. "We didn't know what we had," Mezzacappa said.

The TSI team partnered with another SciDAC project led by Micah Beck of the University of Tennessee, which developed a new data transfer solution known as logistical networking. Logistical networking software tools allow users to create local storage "depots" or utilize shared storage depots deployed worldwide to easily accomplish long-haul data transfers,

temporary storage of large datasets (on the order of terabytes) and prepositioning of data for fast on-demand delivery.

The group provided the hardware and software needed to create a private network linking Oak Ridge and North Carolina State, allowing the data to be moved to the university. There, Blondin used a visualization cluster to analyze and visualize the data, allowing the team to pursue the 3D science. The TSI network now spans the U.S., linking the two original sites with facilities like the National Energy Research Scientific Computing Center in California to the State University of New York at Stony Brook. As the TSI project demonstrated the benefits of logistical networking, researchers in the fusion and combustion communities also built their own logistical networks.

Once the data from the 3D simulations could be analyzed, the team made another discovery that was not possible in the two-dimensional simulations. Once a core-collapse supernova explodes, what remains is known as a neutron star. In some cases, this neutron star spins and emits radiation as light and is called a pulsar. What is not known, however, is what causes a neutron star to get spun up.

A previous theory held that neutron star spin is generated when the stellar core spins up as it collapses during the supernova, much like an ice skater who increases his rotational speed by pulling his arms close to his body. But this simple model cannot explain all the observed characteristics of pulsars and at the same time explain the predicted characteristics of stars at the onset of collapse.

In TSI's 3D models, the SASI produces two counter-rotating flows between the proto-neutron star and the propagating shock wave. As the innermost flow settles onto the proto-neutron star, it imparts angular momentum and causes it to spin, just as you can spin a bicycle tire by swiping your hand across the tread. The team computed their spin predictions and found that the results were within the observed range of pulsars spins.

"This was another breakthrough made possible by SciDAC," Mezzacappa said. "It gives us new possibilities for explaining the spins of pulsars."

The key to their results in both cases, Mezzacappa noted, was scaling their application to simulate complex phenomena in 3D, rather than two dimensions. "In other scientific articles, supernova researchers have written that they don't see much difference between simulations in 2D and 3D, but now we know they are very different, and have shown how this difference is related to the supernova mechanism and byproducts," Mezzacappa said. "Mother Nature clearly works in a 3D universe."

CCSM:

Advanced Simulation Models for Studying Global Climate Change

One of the most widely discussed scientific questions of the past 20 years is the issue of global climate change. But it's not just a matter of science. The question of global climate change also involves economic, environmental, social and political implications. In short, it's a complex question with no easy answers. But detailed climate modeling tools are helping researchers gain a better understanding of how human activities are influencing our climate.

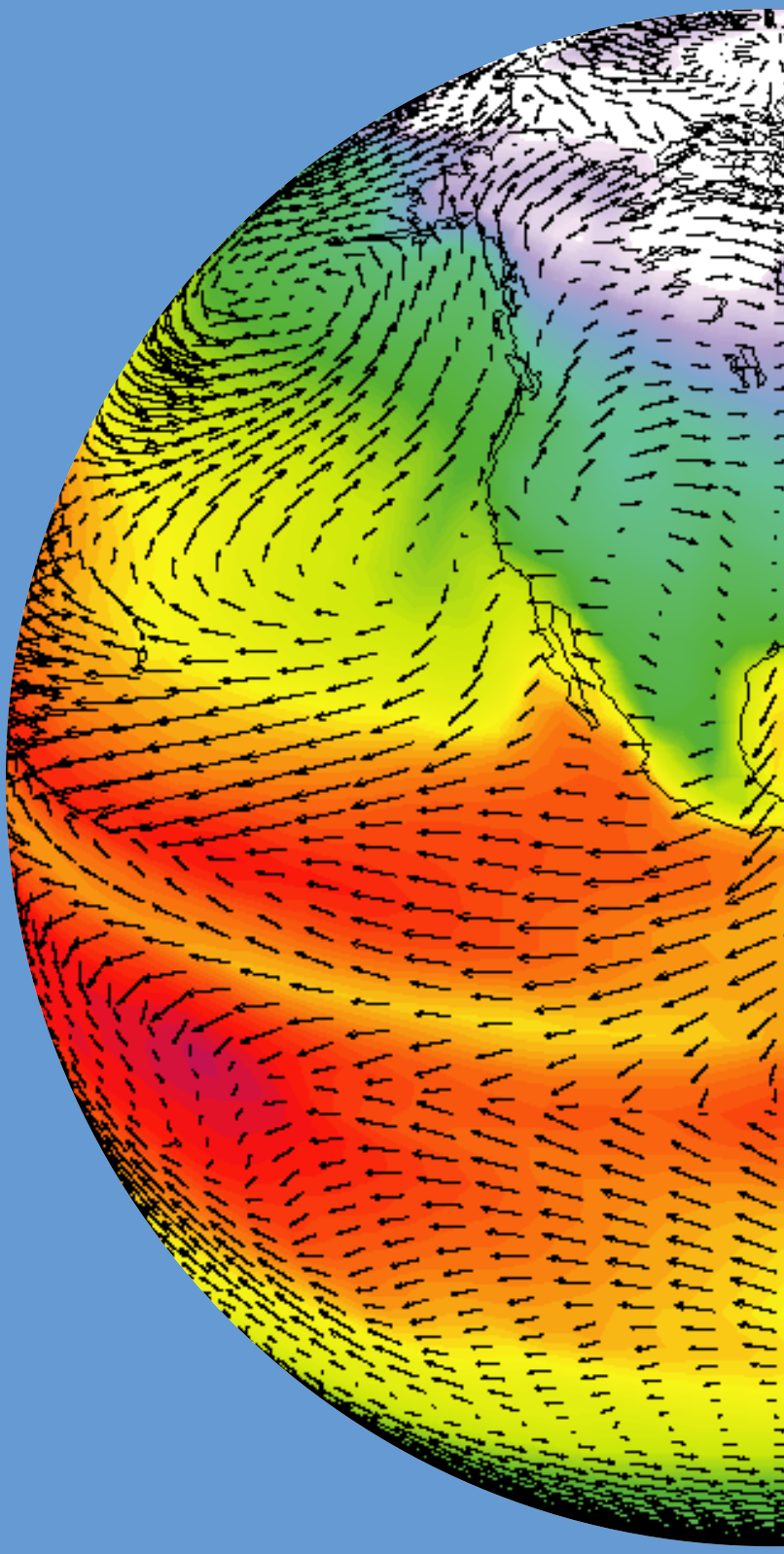
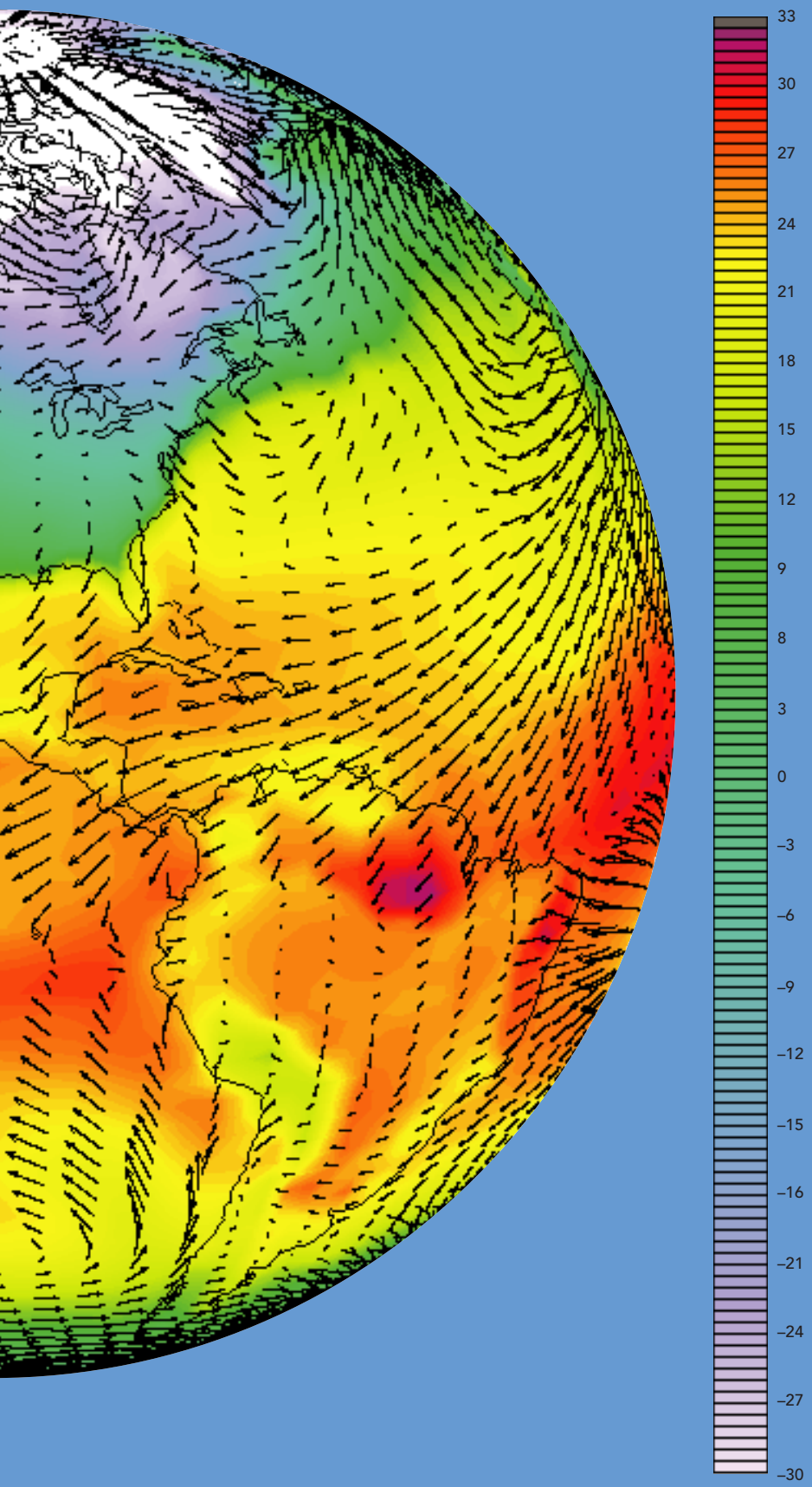


FIGURE 1. Surface temperature (in °C) averaged over December of year 9 of the fully coupled chemistry simulation. Vectors represent the surface wind.



To try to ensure that decision-makers around the world have access to the most accurate information available, the Intergovernmental Panel on Climate Change (IPCC) was established in 1988 under the auspices of the World Meterological Organization and the United Nations Environment Program. The role of the IPCC is to assess on a comprehensive, objective, open and transparent basis the scientific, technical and socio-economic information relevant to understanding the scientific basis of risk of human-induced climate change, its potential impacts and options for adaptation and mitigation.

In accordance with its mandate, the major activity of the IPCC is to prepare at regular intervals comprehensive and up-to-date assessments of relevant for the understanding of human induced climate change, potential impacts of climate change and options for mitigation and adaptation. The First Assessment Report was completed in 1990, the Second Assessment Report in 1995 and the Third Assessment Report in 2001. The Fourth Assessment Report is scheduled to be completed in 2007. SciDAC-sponsored research has enabled the United States climate modeling community to make significant contributions to this report. In fact, the United States is the largest contributor of climate modeling data to the report, as compared to the 2001 report in which no U.S.-generated data was included.

Two large multi-laboratory SciDAC projects are directly relevant to the activities of the IPCC. The first, entitled "Collaborative Design and Development of the Community Climate System Model for Terascale Computers," has made important software contributions to the recently released third version of the Community Climate System Model (CCSM3.0), developed by the National Center for Atmospheric Research, DOE laboratories and the academic community. The second project, entitled "Earth System Grid

II: Turning Climate Datasets into Community Resources," aims to facilitate the distribution of the copious amounts of data produced by coupled climate model integrations to the general scientific community.

A key chapter in the Fourth Assessment Report will look at Global Climate Projections, which will examine climate change to the year 2100 and beyond. Gerald Meehl, one of two lead authors of the chapter and a scientist at the National Center for Atmospheric Research in Colorado, ran extensive simulations using the CCSM and another climate modeling application, PCM, to project climate change through the end of the 21st century.

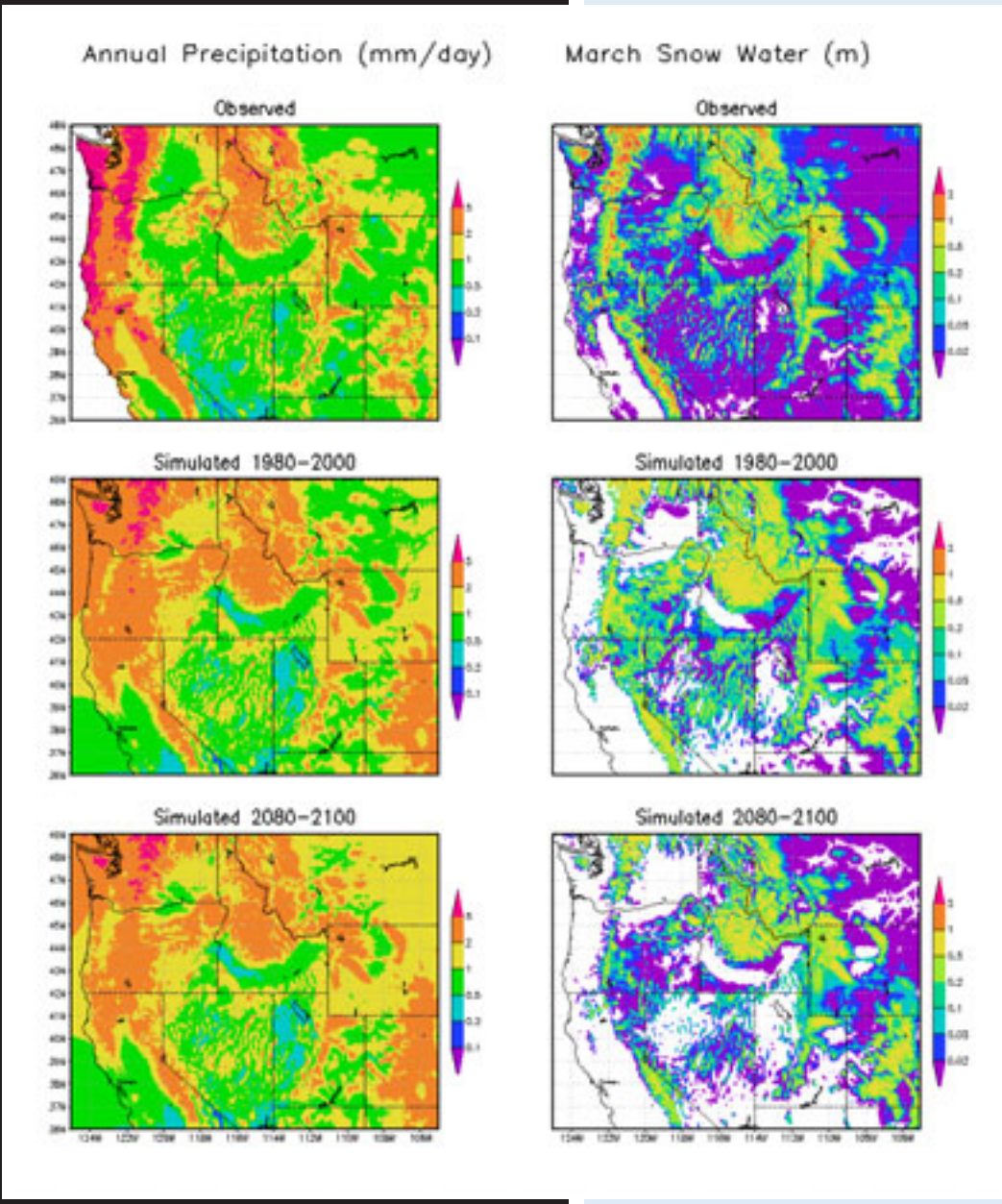


FIGURE 2. Annual precipitation and March snow water from an IPCC simulation using the subgrid orography scheme in Ghan and Shippert (2005).

The results, reported in the March 18, 2005 issue of *Science* magazine, indicate that "even if the concentrations of greenhouse gases in the atmosphere had been stabilized in the year 2000, we are already committed to further global warming of about another half degree and an additional 320 percent sea level rise caused by thermal expansion by the end of the 21st century. … At any given point in time, even if concentrations are stabilized, there is a commitment to future climate changes that will be greater than those we have already observed."

As one of many research organizations from around the world providing input for the IPCC report, the DOE Office of Science is committed to providing data that is as scientifically accurate as possible. This commitment to scientific validity is a key factor behind the SciDAC program to refine and improve climate models.

In order to bring the best science to bear on future climate prediction, modelers must first try to accurately simulate the past. The record of historical climate change is well documented by weather observations and measurements starting around 1890. So, after what is known about the physics and mathematics of atmospheric and ocean flows is incorporated in a simulation model running on one of DOE's supercomputers, the model is tested by "predicting" the climate from 1890 to the present.

The input to such a model is not the answer, but rather a set of data describing known climate conditions – what the atmospheric concentrations of greenhouse gases were, what solar fluctuations occurred, and what volcanic eruptions took place. While past climate models were not able to replicate the historical record with its natural and induced variability, the present generation of coupled ocean, atmosphere, sea ice, and land compo-

nents do a remarkably good job of predicting the past century's climate. This accuracy gives confidence that when the same model is used to generate predictions into the future based on various emission scenarios, the results will have a strong scientific basis and are more than scientific opinions of what might happen.

The Community Climate System Model, CCSM3, is centered at NCAR, arguably a world leader in the field of coupled climate models. This model continues to be developed jointly by the National Science Foundation and DOE to capture the best scientific understanding of climate. In addition to being used for climate change studies, the CCSM is being used to study climate-related questions ranging from ancient climates to the physics of clouds. However, the DOE national laboratories and the National Center for Atmospheric Research periodically use the model for assessment purposes such as the IPCC project.

The SciDAC CCSM Consortium developing the model has also made sure that it runs effectively on the most powerful supercomputers at DOE's leading computing centers – the Leadership Class Facility (LCF) in Tennessee and the National Energy Research Scientific Computing Center (NERSC) in California. DOE contributed significant allocations of supercomputer time to the international efforts (along with NCAR and the Japanese Earth Simulator Center) toward the completion of the IPCC runs with CCSM3.

The fruit of these labors is substantial. Enabled by these sizable allocations, the CCSM3 is the largest single contributor to the IPCC Assessment Report 4 database. Not only is the model represented in more transient scenarios than any other model, more statistically independent realizations of each of these scenarios have been integrated than with any other model. Also, the resolution of the atmosphere component is exceeded by only one other model (which has not been ensemble-integrated).

This increase in production is scientifically important in many ways. The need for large numbers of individual simulations is especially important when attempting to characterize the uncertainty of climate change. For instance, in looking at recent climate change (over the last century), running more statistically independent simulations of the 20th century allows researchers to produce a much better defined pattern of climate changes. To model future climate change, scientists will run multiple simulations with a given level of greenhouse gas emissions to quantify the range of possible outcomes. And when researchers want to study possible outcomes for a range of emissions, they need to run even more simulations.

Running simulations for extended times are also important to help researchers detect and take into account conditions which result from flaws in the climate model. Such flaws cause "drift," or an unsubstantiated change in temperature. While drift-free control runs covering several hundred years are useful for studying climate change over a few decades, examining climate change of the entire 20th century requires a control run of at least 1,000 years to avoid misinterpretation of the resulting climate model. In summary, large ensembles and long control runs are necessary to better understand the clear patterns of climate change.

Through SciDAC, DOE also sponsors the technology being used to make available the results to scientists worldwide. The Earth System Grid (ESG) project collects all the data from all the runs of models in the U.S., as well as from other countries, and makes the data accessible to scientists throughout the world. This allows scientists in the international climate research community to analyze more extensive datasets, compare results and document differences in model predictions. In fact, over 200 papers are in press referencing this data. (You can see a list at http://www-pcmdi.llnl.gov/ipcc/diagnostic_subprojects.php.)

When researchers encounter disagreement among models, scientific debates and discussions ensue about the physical mechanisms governing the dynamics of climate. This debate is typically vigorous and points in directions that models can be improved. To take advantage of such discussions and to improve the validity of climate models, DOE sponsors the Program for Model Intercomparison and Diagnosis (PCMDI), which places the scientific basis of climate modeling front and center in its work. Such rigorous peer review and discussion is critical to ensuring that government officials have access to the most scientifically valid information when making decisions regarding climate change.

This SciDAC project is a collaboration between six DOE National Laboratories (ANL, LANL, LBNL, LLNL, ORNL, PNNL) and NCAR. The lead investigators representing these institutions are R. Jacob, P. Jones, C. Ding, P. Cameron-Smith, J. Drake, S. Ghan, W. Collins, W. Washington and P. Gent.

Plasma Physics

Terascale Simulations Predict Favorable Confinement Trend for Reactor-Scale Plasmas

Most people do not think about turbulence very often, except when they are flying and the captain turns on the "Fasten Seat Belts" sign. The kind of turbulence that may cause problems for airplane passengers involves swirls and eddies that are a great deal larger than the aircraft. But in fusion plasmas, much smaller-scale turbulence, called microturbulence, can cause serious problems–specifically, instabilities and heat loss that could stop the fusion reaction.

In fusion research, all of the conditions necessary to keep a plasma dense and hot long enough to undergo fusion are referred to as confinement. The retention of heat, called energy confinement, can be threatened by microturbulence, which can make particles drift across, rather than along with, the plasma flow. At the core of a fusion reactor such as a tokamak, the temperatures and densities are higher than at the outside edges. As with weather, when there

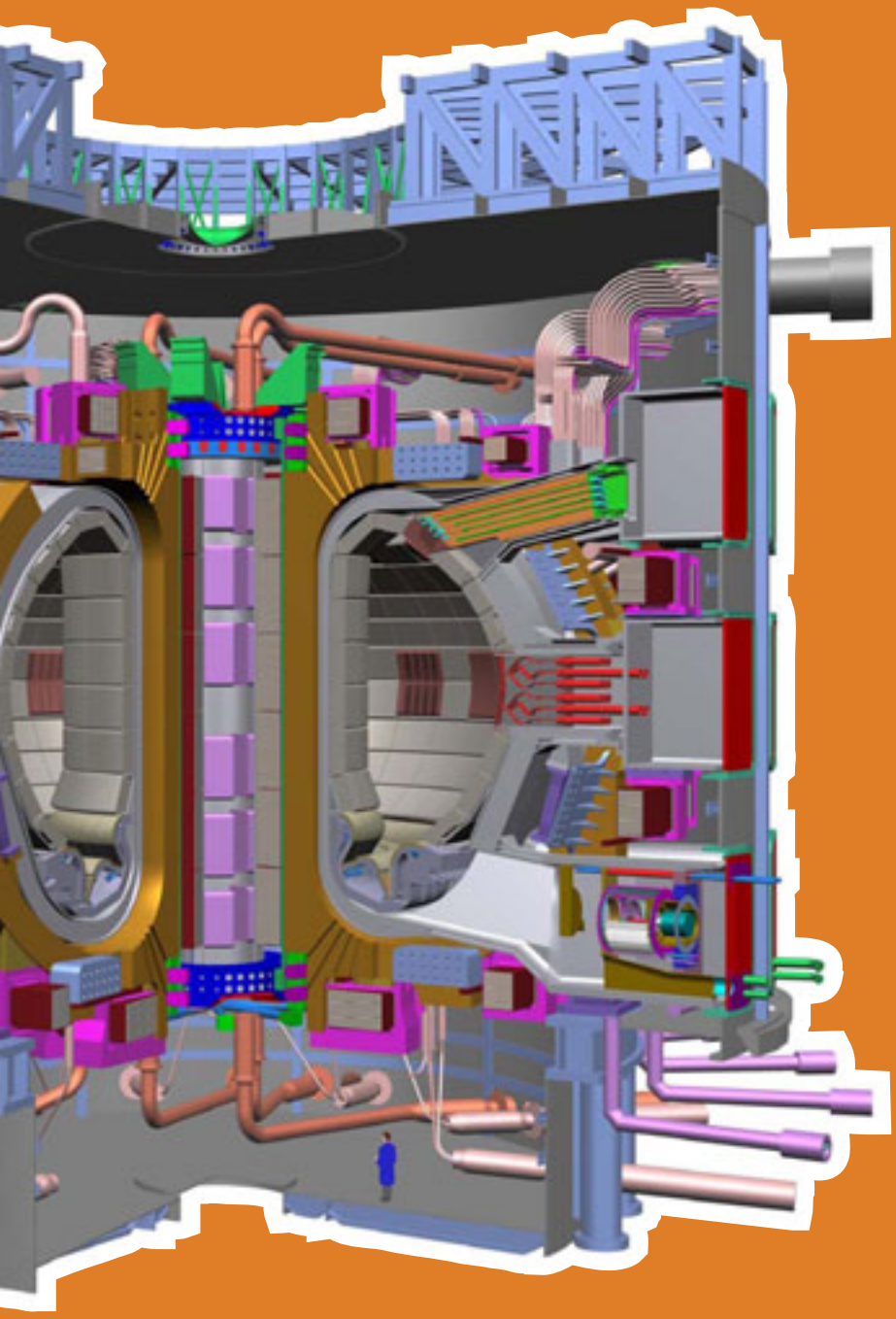


FIGURE 1. Cutaway illustration of the ITER tokamak.

are two regions with different temperatures and densities, the area between is subject to turbulence. In a tokamak, turbulence can allow charged particles in the plasma to move toward the outer edges of the reactor rather than fusing with other particles in the core. If enough particles drift away, the plasma loses temperature and the fusion reaction cannot be sustained.

One troublesome result of tokamak experiments to date is that as the size of the plasma increases, the relative level of heat loss from turbulent transport also increases. Because the size (and therefore cost) of a fusion experiment is determined largely by the balance between fusion self-heating and turbulent transport losses, understanding this process is of utmost importance for the design and operation of fusion devices such as the multi-billion-dollar ITER project. ITER (Latin for "the way"), a multinational tokamak experiment to be built at Cadarache in southern France, is one of the highest strategic priorities of the DOE Office of Science.

Underlining America's commitment to ITER, U.S. Energy Secretary Samuel Bodman stated on June 28, 2005, "Plentiful, reliable energy is critical to worldwide economic development. Fusion technologies have the potential to transform how energy is produced and provide significant amounts of safe, environmentally friendly power in the future. The ITER project will make this vision a reality."

ITER is expected to produce 500 million thermal watts of fusion power–10 times more power than is needed to heat the plasma–when it reaches full operation around the year 2016. As the world's first production-scale fusion reactor (Figure 1), ITER will help answer questions about the most efficient ways to configure and operate future commercial reactors.

The growth of the microinstabilities that lead to turbulent transport has been extensively studied over the years, not only because understanding this process is an important practical problem, but also because it is a true scientific grand challenge which is particularly well suited to be addressed by modern terascale computational resources. And the latest news, confirmed by multiple simulations using different codes, is good: in reactors the size of ITER, heat losses caused by plasma turbulence no longer follow the empirical trend of increasing with the size of the plasma. Instead, the rate of heat loss levels off and stabilizes.

Progress in understanding plasma ion dynamics has been impressive. For example, studies show that electrostatic ion temperature gradient (ITG) driven turbulence can be sup-

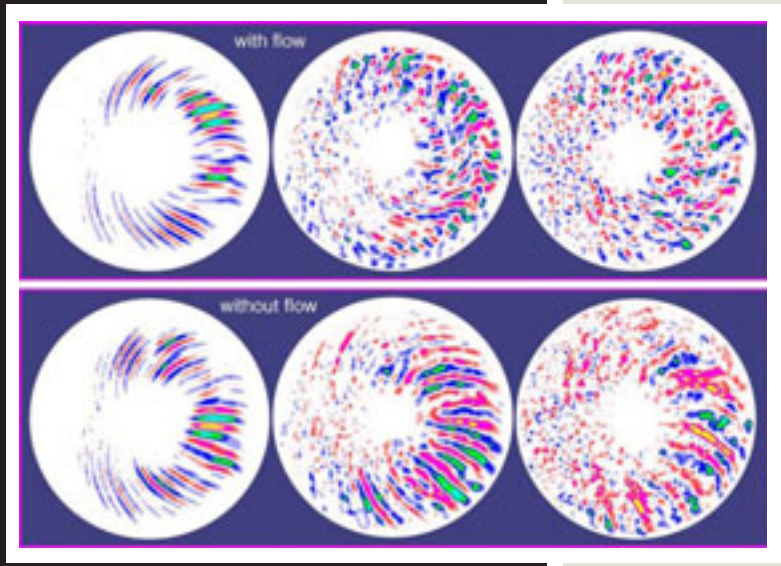


FIGURE 2. Turbulence reduction via sheared plasma flow compared to case with flow suppressed.

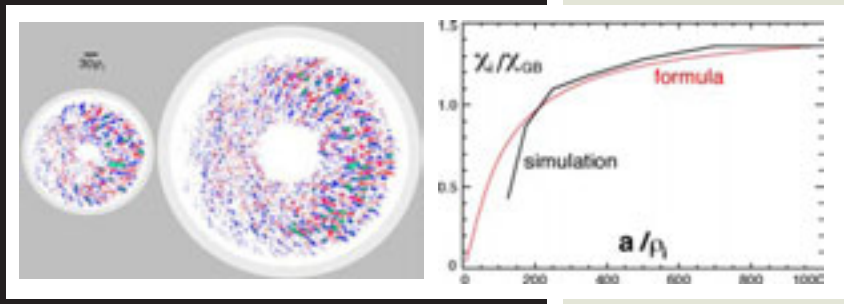


FIGURE 3. Full torus particle-in-cell gyrokinetic simulations (GTC) of turbulent transport scaling. (Left) The granular structures represent the scales of the turbulence in a typical plasma which need to be included in realistic plasma simulations. (Right) The horizontal axis expresses the plasma size, and the point at 1000 represents ITER's size. The vertical axis represents the thermal diffusion, or heat loss.

pressed by self-generated zonal flows within the plasma. The suppression of turbulence is caused by a shearing action that destroys the finger-like density contours which promote thermal transport. This dynamic process is depicted by the sequences shown in Figure 2, obtained using the Gyrokinetic Toroidal Code (GTC) developed by the SciDAC-funded Gyrokinetic Particle Simulation Center (GPSC). The lower panels show the nonlinear evolution of the turbulence in the absence of flow, while the upper panels illustrate the turbulence decorrelation caused by the self-generated "E×B" flow, which arises from crossed electric and magnetic fields.

This simulation is a good example of the effective use of powerful supercomputers (in this case, the 10 teraflop/s Seaborg IBM SP at NERSC). Typical global particle-in-cell simulations of this type have used one billion particles with 125 million grid points over 7000 time steps to produce significant physics results. Simulations of this size would not be feasible on smaller computers.

Large-scale simulations have also explored key consequences of scaling up from present-day experimental fusion devices (around 3 meters radius for the largest existing machines) to ITER-sized reactors (about 6 meters). For the reactor-scale plasmas of the future, these simulations suggest that the relative level of heat loss driven by electrostatic ITG turbulence does not increase with plasma size (Figure 3). This transition from "Bohm" (linear) scaling to "gyro-Bohm" (quadratic) scaling is a positive trend, because simple empirical extrapolation of the smaller system findings would produce much more pessimistic predictions for energy confinement. Since neither experiments nor theory and simulations have previously been able to explore such trends in an ITER-sized plasma, these results represent a significant scientific discovery enabled by the SciDAC program.

Exploration of the underlying causes for the transition in the rate of heat loss that simulations show around the 400 gyroradii range has inspired the development of new nonlinear theoretical models based on the spreading of turbulence. Although this predicted trend is a very favorable one, the fidelity of the analysis needs to be further examined by investigating additional physics effects, such as kinetic electromagnetic dynamics, which might alter the present predictions.

The excellent scaling of the GTC code provides strong encouragement that future simulations will be able to capture the additional complexity and lead to greater scientific discoveries. GTC is currently involved in benchmark tests on a variety of supercomputing platforms–including the Earth Simulator in Japan, the Cray X1E and XT line at Oak Ridge National Laboratory, the IBM Power SP line, and the IBM Blue Gene line–and exhibits scaling properties which look to be readily extensible to the peta-scale regime. GTC's performance and scaling on a variety of leading platforms is illustrated in Figure 4.

The GS2 and GYRO codes developed by the Plasma Microturbulence Project (the SciDAC predecessor to the current GPSC) have also contributed productively to the interpretation of turbulence-driven transport

trends observed in experiments. These two SciDAC projects have involved researchers from Lawrence Livermore National Laboratory; Princeton Plasma Physics Laboratory (PPPL); Columbia University; the University of California at Los Angeles, Irvine, and Davis; the University of Colorado; the University of Maryland; the University of Tennessee at Knoxville; Oak Ridge National Laboratory; and General Atomics.

Bill Tang, Chief Scientist at PPPL, is encouraged by the progress in computational fusion research. "SciDAC has contributed strongly to the accelerated development of computational tools and techniques needed to develop predictive models for the analysis and design of magnetically confined plasmas," Tang commented. "Unraveling the complex behavior of strongly nonlinear plasma systems under realistic conditions is a key component of the next frontier of computational plasma physics in general and fusion research in particular. Accelerated progress in the development of the needed codes with higher physics fidelity has been greatly aided by the interdisciplinary alliances championed by the SciDAC Program, together with necessary access to the tremendous increase in compute cycles enabled by the rapid advances in supercomputer technology."

Ray Orbach, Director of the DOE Office of Science, expressed his hope for high-end computing's future contributions to fusion energy in an interview in SciDAC Review (Number 1, Spring 2006, p. 8): "At the speeds that we are talking about [50 teraflop/s], the electrons in a fusion device can be considered as real point particles and do not have to be treated in mean field approximations. So for the first time at 50 TF, one will be able to do simulations of high-density, high-temperature plasmas that were never possible before. This will have a significant impact on the treatment of these highly nonlinear systems. These systems are not subject to analytic examination and there may be instabilities that no one has thought about. This has already been found to be of profound importance for ITER [and] for fusion science in general."

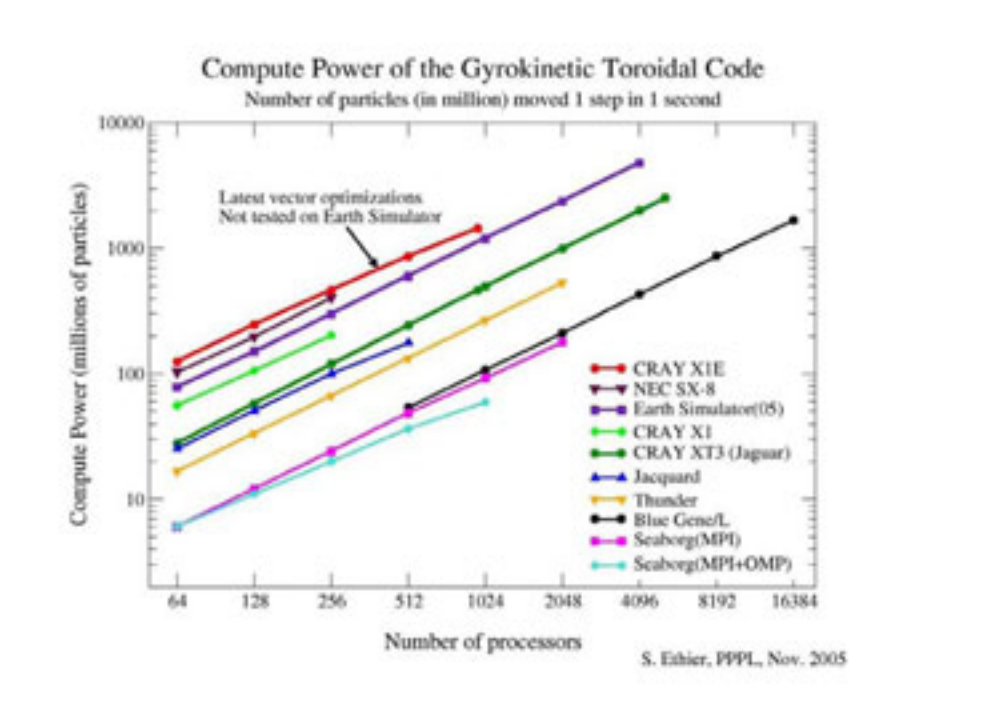
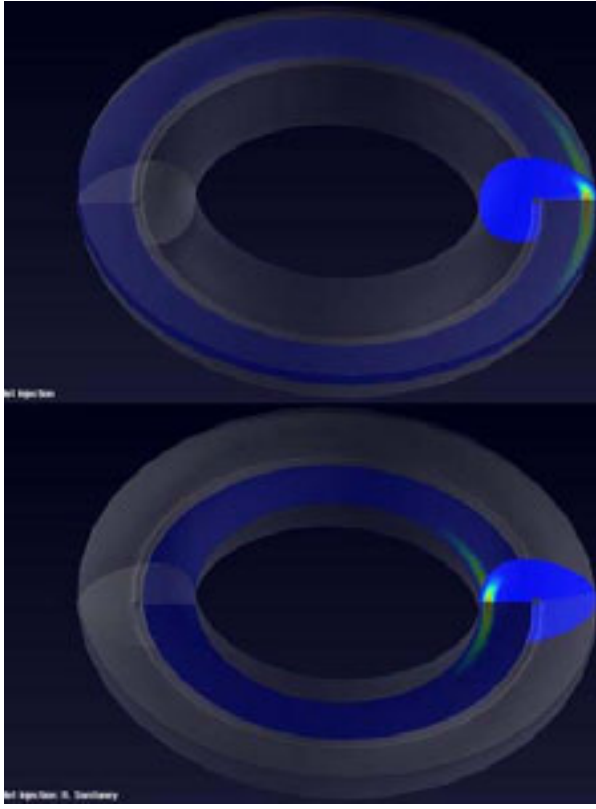


Figure 4. Scaling study of the GTC code on multiple high performance computing platforms.

Hailstones in hell

Simulations Examine the Behavior of Frozen Fuel Pellets in Fusion Reactors



What happens when you shoot one of the coldest materials into the hottest environment on earth? The answer may help solve the world's energy crisis.

Imagine that there is a large chamber in hell that's shaped like a doughnut, and that you'd like to shoot a series of hailstones into that chamber so that as they melt, the water vapor penetrates as deeply as possible and disperses as evenly as possible throughout the chamber. Setting aside for a moment the question of *why* you would want to do that, consider the multitude of *how* questions: Should you shoot in the hailstones from outside the ring of the doughnut or from inside the hole? What size hailstones should you use? At what speed and angle should they enter the chamber?

This strange scenario is actually an analogy for one of the questions facing fusion energy researchers: how to refuel a tokamak. A tokamak is a machine that produces a toroidal (doughnut-shaped) magnetic field. In that field, two isotopes of hydrogen – deuterium and tritium – are heated to about 100 million degrees Celsius (more than six times hotter than the interior of the sun), stripping the electrons from the nuclei. The magnetic field makes the electrically charged particles follow spiral paths around the magnetic field lines, so that they spin around the torus in a

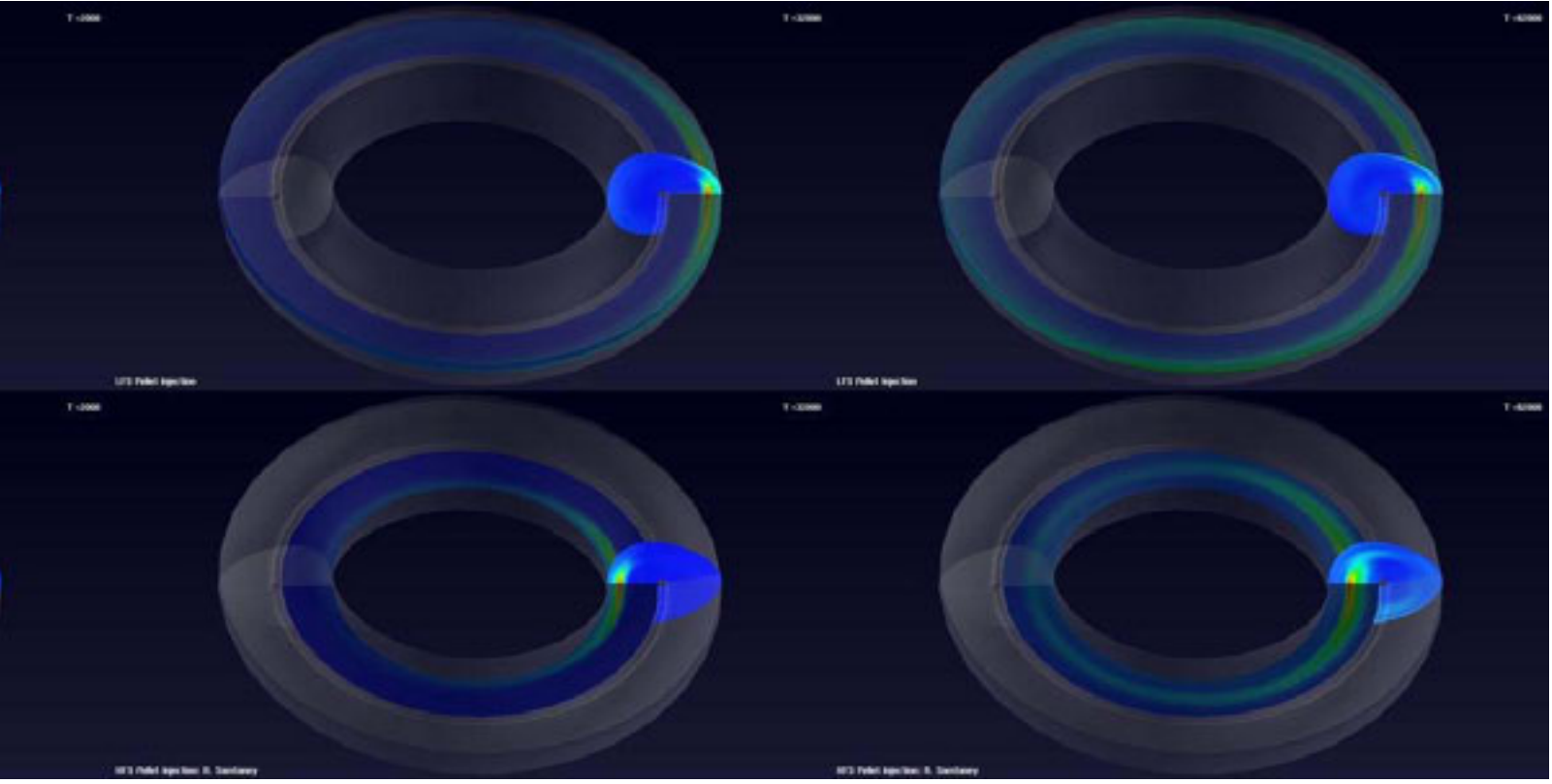


FIGURE 1. These simulations show the results of pellet injection into a tokamak fusion reactor from the low-field-side (LFS) and high-field-side (HFS). The top row shows a time sequence of the density in LFS injection while the bottom panel shows density evolution in HFS injection. The dominant motion of the ablated pellet mass is along field lines accompanied by transport of material across flux surfaces towards the low field side. This observation is qualitatively consistent with experimental observations leading to the conclusion that HFS pellet injection is a more efficient refueling technique than LFS injection. The MHD instabilities which cause the pellet material to move towards the low field side are currently under investigation.

fairly uniform flow and interact with each other, not with the walls of the tokamak. When the hydrogen ions (nuclei) collide at high speeds, they fuse, releasing energy. If the fusion reaction can be sustained long enough that the amount of energy released exceeds the amount needed to heat the plasma, researchers will have reached their goal: a viable energy source from abundant fuel that produces no greenhouse gases and no long-lived radioactive byproducts.

High-speed injection of frozen hydrogen pellets is an experimentally proven method of refueling a tokamak. These pellets are about the size of small hailstones (3–6 mm) and have a temperature of about 10 degrees Celsius above absolute zero. The goal is to have these pellets penetrate as deeply as possible into the plasma so that the fuel disperses evenly.

Pellet injection will be the primary fueling method used in ITER (Latin for "the way"), a multinational tokamak experiment to be built at Cadarache in southern France. ITER, one of the highest strategic priorities of the DOE Office of Science, is expected to produce 500 million thermal watts of fusion power – 10 times more power than is needed to heat the plasma – when it reaches full operation around the year 2016. As the world's first production-scale fusion reactor, ITER will help answer questions about the most efficient ways to configure and operate future commercial reactors.

However, designing a pellet injection system that can effectively deliver fuel to the interior of ITER represents a special challenge because of its unprecedented large size and high temperatures. Experiments have shown that a pellet's penetration distance into the plasma depends strongly on how the injector is oriented in relation to the torus. For example, an "inside launch" (from inside the torus ring) results in better fuel distribution than an "outside launch" (from outside the ring).

In the past, progress in developing an efficient refueling strategy for ITER has required lengthy and expensive experiments. But thanks to a three-year, SciDAC-funded collaboration between the Computational Plasma Physics Theory Group at Princeton Plasma Physics Laboratory and the Advanced Numerical Algorithms Group at Lawrence Berkeley National Laboratory, computer codes have now reproduced some key experimental findings, resulting in significant progress toward the scientific goal of using simulations to predict the results of pellet injection in tokamaks.

"To understand refueling by pellet injection, we need to understand two phases of the physical process," said Ravi Samtaney, the Princeton researcher who is leading the code development effort. "The first phase is the transition from a frozen pellet to gaseous hydrogen, and the second phase is the distribution of that gas in the existing plasma."

The first phase is fairly well

understood from experiments and theoretical studies. In this phase, called ablation, the outer layer of the frozen hydrogen pellet is quickly heated, transforming it from a solid into an expanding cloud of dense hydrogen gas surrounding the pellet. This gas quickly heats up, is ionized, and merges into the plasma. As ablation continues, the pellet shrinks until all of it has been gasified and ionized.

The second phase – the distribution of the hydrogen gas in the plasma – is less well understood. Ideally, the injected fuel would simply follow the magnetic field lines and the "flux surfaces" that they define, maintaining a stable and uniform plasma pressure. But experiments have shown that the high-density region around the pellet quickly heats up to form a local region of high pressure, higher than can be stably confined by the local magnetic field. A form of "local instability" (like a mini-tornado) then develops, causing the high-density region to rapidly move across, rather than along, the field lines and flux surfaces – a motion referred to as "anomalous" because it deviates from the large-scale motion of the plasma.

Fortunately, researchers have discovered that they can use this instability to their advantage by injecting the pellet from inside the torus ring, because from this starting point, the anomalous motion brings the fuel pellet closer to the center of the plasma, where it does the most good. This anomalous motion is one of the phenomena that Samtaney and his colleagues want to quantify and examine in detail.

Figure 3 shows the fuel distribution phase as simulated by Samtaney and his colleagues in the first detailed 3D calculations of pellet injection. The inside launch (top row) distributes the fuel in the central region of the plasma, as desired, while the outside launch (bottom row) disperses the fuel near the plasma boundary, as shown in experiments.

Simulating pellet injection in 3D is difficult because the physical processes span several decades of time and space scales. The large disparity between pellet size and tokamak size, the large density differences between the pellet ablation cloud and

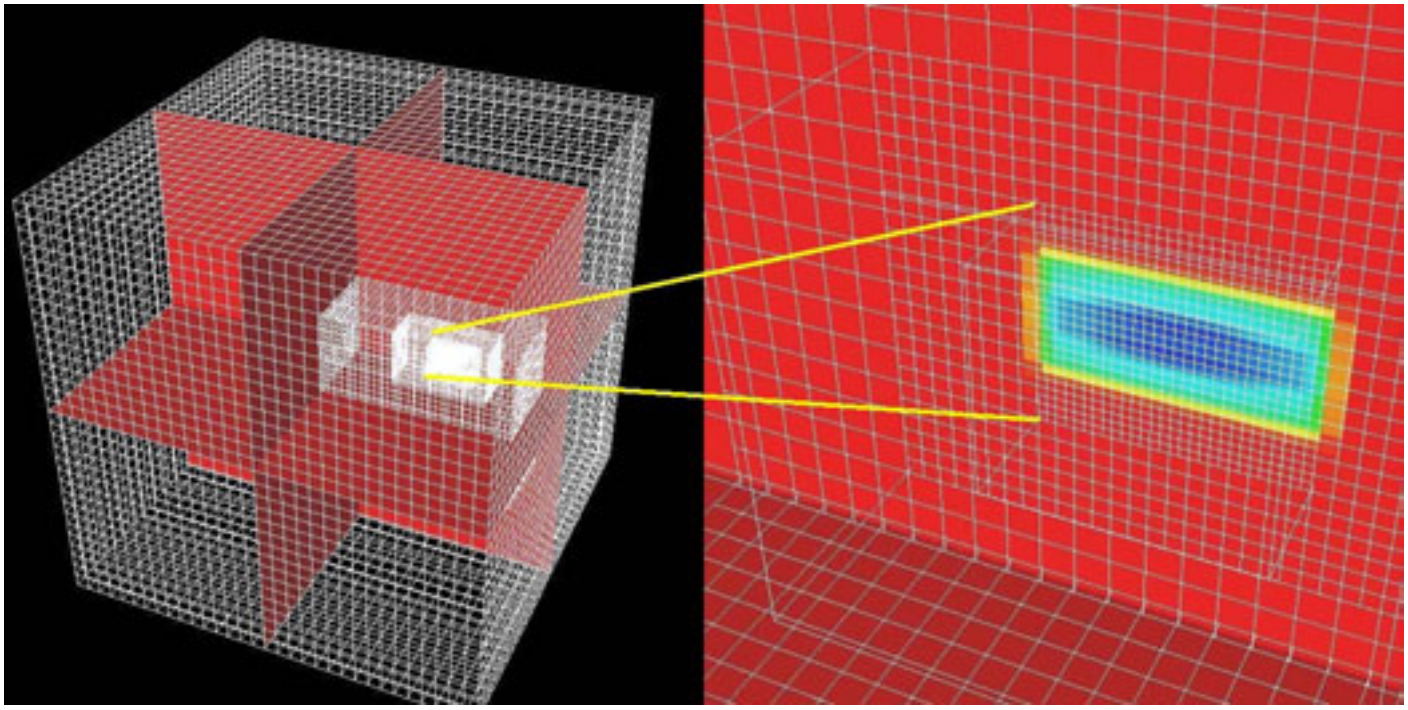


FIGURE 2. This illustration shows how computational problems are solved by dividing them into smaller pieces by covering them with a mesh. In this case, the fuel pellet for a fusion reactor is buried within the finest mesh which occupies less than 0.015 percent of the volume of the coarsest mesh. Using a technique known as adaptive mesh refinement, scientists can focus the power of a supercomputer on the most interesting part of a problem, such as the fuel pellet in a hot plasma.

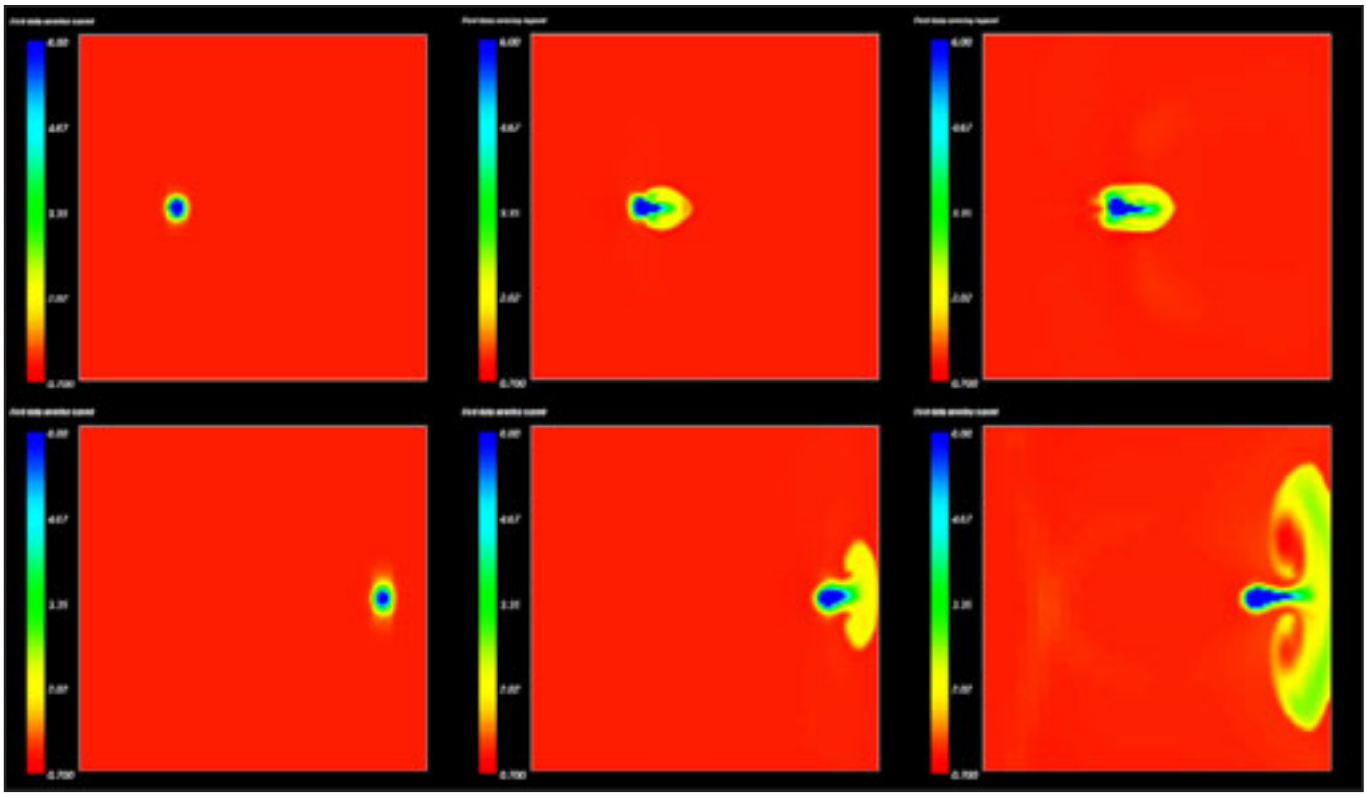


FIGURE 3. Time sequence of 2D slices from a 3D simulation of the injection of a fuel pellet into a tokamak plasma. Injection from outside the torus (bottom row, injection from right) results in the pellet stalling and fuel being dispersed near the plasma boundary. Injection from inside the torus (top row, injection from left) achieves fuel distribution in the hot central region as desired.

the ambient plasma, and the long-distance effects of electron heat transport all pose severe numerical challenges. To overcome these difficulties, Samtaney and his collaborators used an algorithmic method called adaptive mesh refinement (AMR), which incorporates a range of scales that change dynamically as the calculation progresses. AMR allowed this simulation to run more than a hundred times faster than a uniform-mesh simulation.

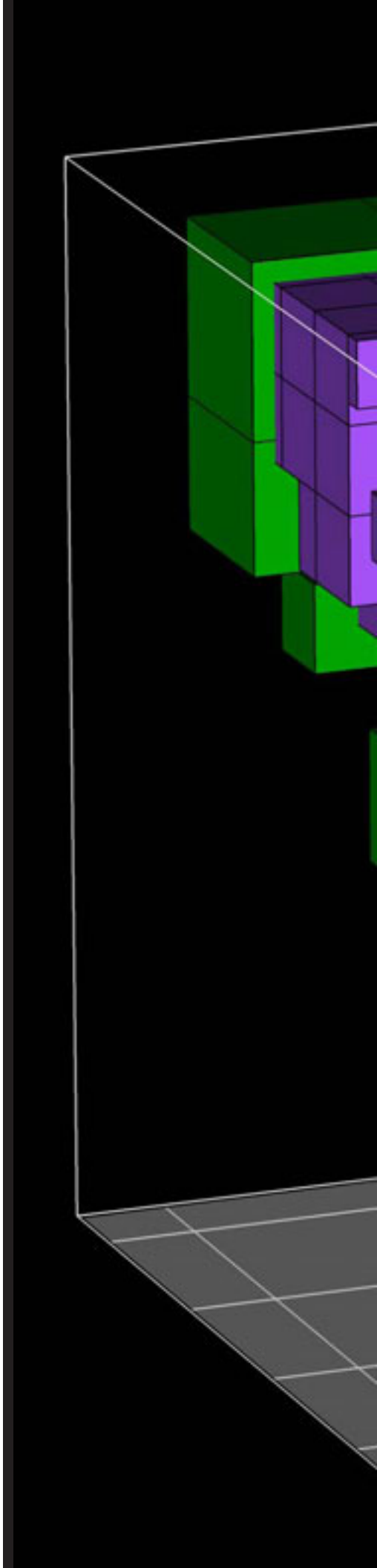
While these first calculations represent an important advance in methodology, Samtaney's work on pellet injection is only beginning. "The results presented in this paper did not include all the detailed physical processes which we're starting to incorporate, along with more realistic physical parameters," he said. "For example, we plan to develop models that incorporate the perpendicular transport of the ablated mass. We also want to investigate other launch locations. And, of course, we'll have to validate all those results against existing experiments."

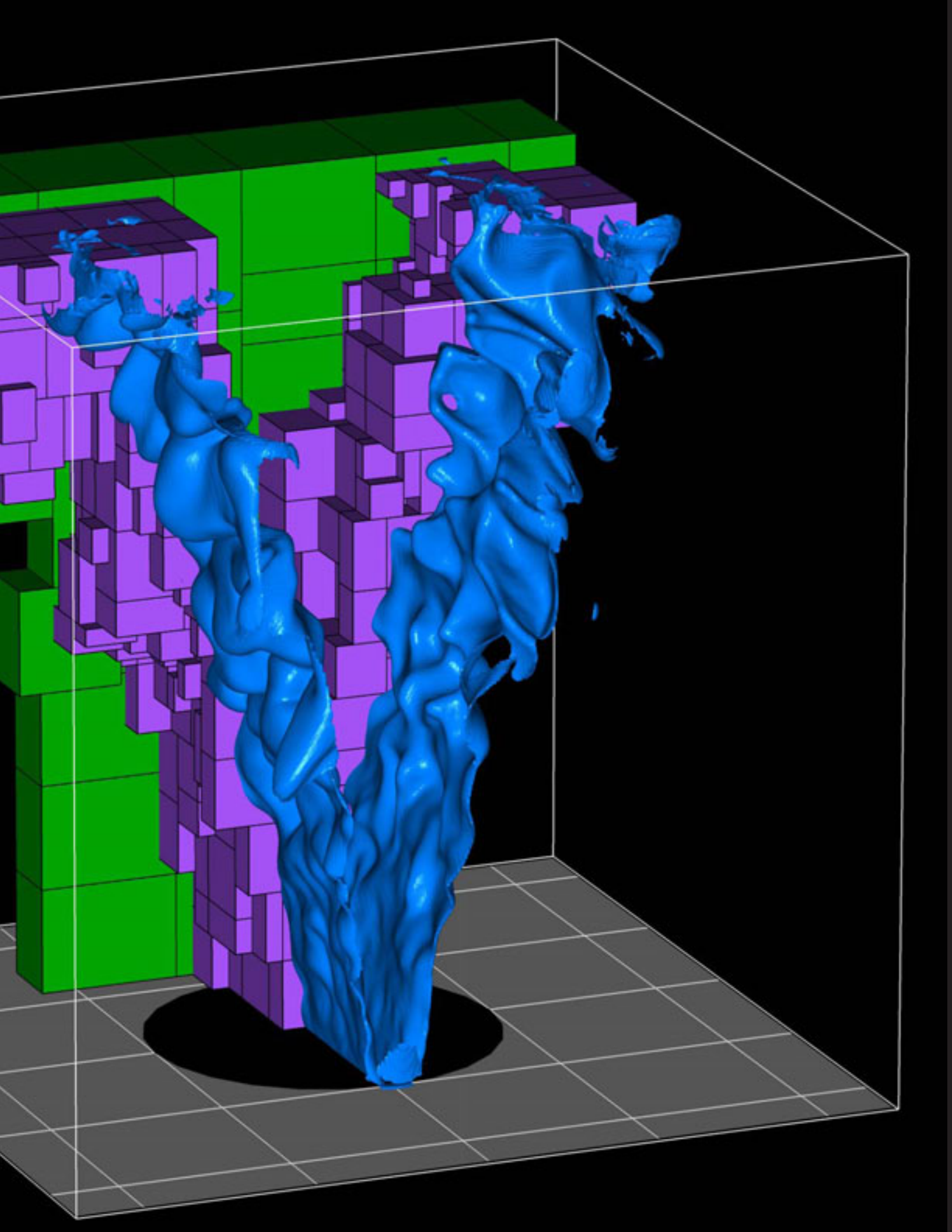
This pellet injection model will eventually become part of a comprehensive predictive capability for ITER, which its supporters hope will bring fusion energy within reach as a commercial source of electrical power.

Burning questions

New 3D Simulations Are Closing in on the Holy Grail of Combustion Science: Turbulence–Chemistry Interactions

Controlling fire to provide heat and light was one of humankind's first great achievements, and the basic chemistry of combustion – what goes in and what comes out – was established long ago. But a complete quantitative understanding of what happens during the combustion process has remained as elusive as the ever-changing shape of a flame.





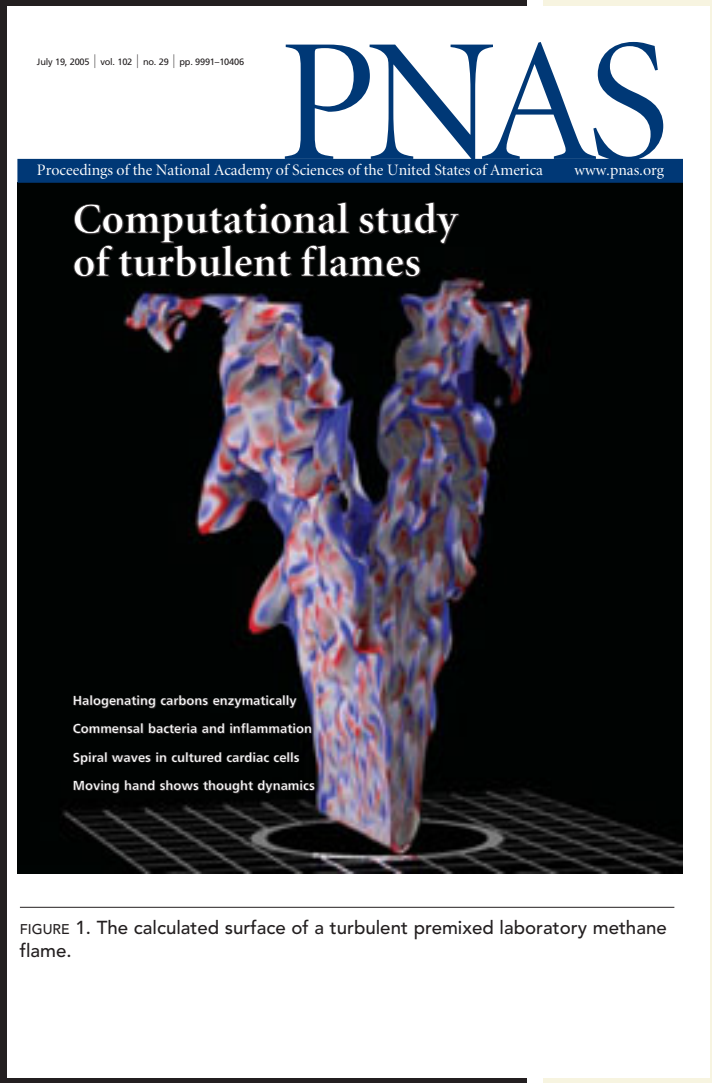


FIGURE 1. The calculated surface of a turbulent premixed laboratory methane flame.

Even a simple fuel like methane (CH_4), the principal component of natural gas, burns in a complex sequence of steps. Oxygen atoms gradually replace other atoms in the hydrocarbon molecules, ultimately leaving carbon dioxide and water. Methane oxidation involves about 20 chemical species for releasing energy, as well as many minor species that can become pollutants. Turbulence can distort the distribution of species and the redistribution of thermal energy which are required to keep the flame burning. These turbulence–chemistry interactions can cause the flame to burn faster or slower and to create more or less pollution.

The holy grail of combustion science has been to observe these turbulence–chemistry effects. Over the past few decades amazing progress has been made in observational techniques, including the use of lasers to excite molecules of a given species and produce a picture of the chemical distribution. But laser imaging is limited in the species and concentrations that can be reliably observed, and it is difficult to obtain simultaneous images to correlate different chemical species.

Because observing the details of combustion is so difficult, progress in combustion science has largely coincided with advances in scientific computing. For example, while basic concepts for solving one-dimensional flat flames originated in the 1950s, it only became possible to solve the 1D flame equations some 30 years later using Cray-1 supercomputers. Those calculations, which are routine on personal computers today, enabled a renaissance in combustion science by allowing chemists to observe the interrelationships among the many hypothesized reaction processes in the flame.

Simulating three-dimensional turbulent flames took 20 more years of advances in applied mathematics, computer science, and computer hardware, particularly massively parallel systems. But the effort has been worth it. New 3D simulations are beginning to provide the kind of detailed information about the structure and dynamics of turbulent flames that will be needed to design new low-emission, fuel-efficient combustion systems.

The first 3D simulation of a laboratory-scale turbulent flame from first principles – the result of a SciDAC-funded collaboration between computational and experimental scientists at Berkeley Lab – was featured on the cover of the July 19, 2005 Proceedings of the National Academy of Sciences (Figure 1). The article, written by John Bell, Marc Day, Ian Shepherd, Matthew Johnson, Robert Cheng, Joseph Grcar, Vincent Beckner, and Michael Lijewski, describes the simulation of "a laboratory-scale turbulent rod-stabilized premixed methane V-flame." This simulation was unprecedented in several aspects – the number of chemical species included, the number of chemical reactions modeled, and the overall size of the flame.

This simulation employed a different mathematical approach than has typically been used for combustion. Most combustion simulations designed for basic research use compressible flow equations that include sound waves, and are calculated with small time steps on very fine, uniform spatial grids – all of which makes them very computationally expensive. Because of limited computer time, such simulations often have been restricted to only two dimensions, to

scales less than a centimeter, or to just a few carbon species and reactions.

In contrast, the Center for Computational Sciences and Engineering (CCSE), under Bell's leadership, has developed an algorithmic approach that combines low Mach-number equations, which remove sound waves from the computation, with adaptive mesh refinement, which bridges the wide range of spatial scales relevant to a laboratory experiment. This combined methodology strips away relatively unimportant aspects of the simulation and focuses computing resources on the most important processes, thus slashing the computational cost of combustion simulations by a factor of 10,000.

Using this approach, the CCSE team has modeled turbulence and turbulence–chemistry interactions for a three-dimensional flame about 12 cm (4.7 in.) high, including 20 chemical species and 84 fundamental chemical reactions. The simulation was realistic enough to be compared directly with experimental diagnostics.

The simulation captured with remarkable fidelity some major features of the experimental data, such as flame-generated outward deflection in the unburned gases, inward flow convergence, and a centerline flow acceleration in the burned gases (Figure 2). The simulation results were found to match the experimental results within a few percent. This agreement directly validated both the computational method and the chemical model of hydrocarbon reaction and transport kinetics in a turbulent flame.

The results demonstrate that it is possible to simulate a laboratory-scale flame in three dimensions without having to sacrifice a realistic representation of chemical and transport processes. This advance has the potential to greatly increase our understanding of how fuels behave in the complicated environments inside turbulent flames.

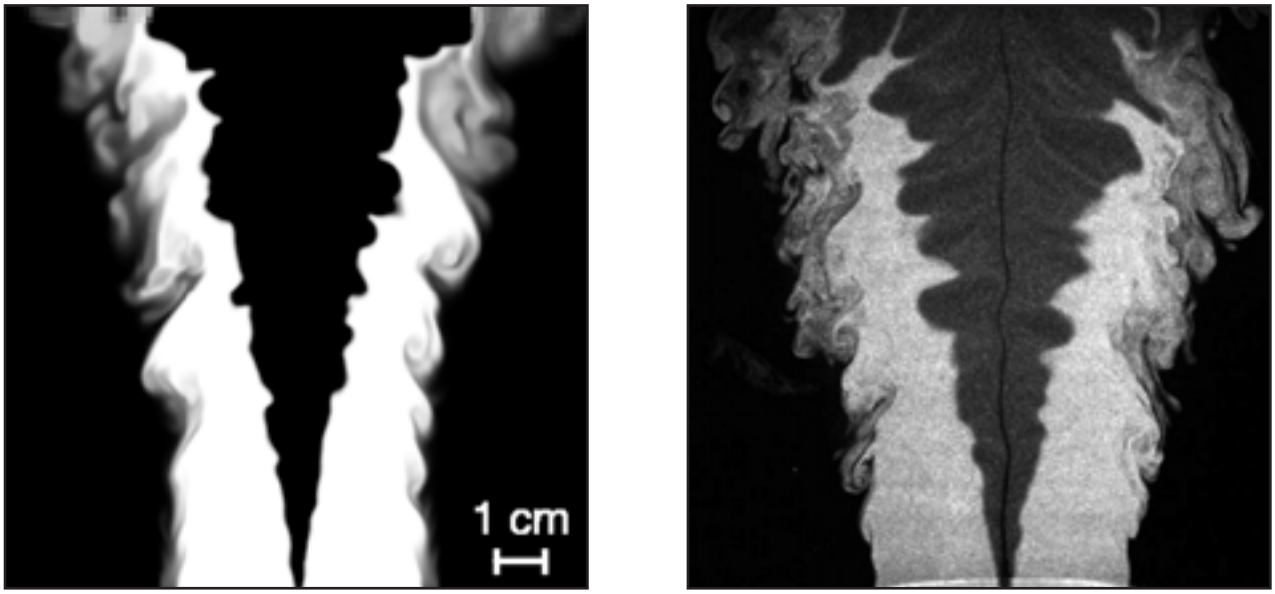


FIGURE 2. Left: A typical centerline slice of the methane concentration obtained from the simulation. Right: Experi-mentally, the instantaneous flame location is determined by using the large differences in Mie scattering intensities from the reactants and products to clearly outline the flame. The wrinkling of the flame in the computation and the experiment is of similar size and structure.

Pushing the Frontiers of Chemistry

Dirac's Vision Realized

In most first-year chemistry classes at universities, students begin by learning how atoms of carbon and other elements form bonds with other atoms to form molecules, which in turn combine to form ourselves, our planet and our universe.

Understanding the properties and behavior of molecules, or better yet, being able to predict and control the behavior, is the driving force behind modern chemistry. The development of the theory of quantum mechanics in the 1920's made it possible that all the properties of molecules could be predicted. One its founders, Paul Dirac, wrote in 1929 that "the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

Almost 80 years later this is still true, even using the most powerful supercomputers. For example, a scientist could solve for the behavior of a molecule with one electron moving in one dimension on a grid of roughly 100 points spread along that line. Since electrons in free space move in three dimensions, not one, the scientist would need 100^3 (one million) calculations. Adding each extra electron then entails about a million times more work, a condition known as exponential scaling, so it is no wonder that the largest exact calculations still involve no more than about 15 electrons. Even with anticipated supercomputing advances over the next decade, only one or maybe two more electrons could be treated this way.

Quantum chemistry, however, provides scientists with the models to approximate these values without doing all the calculations. But there is a tradeoff, since researchers need to balance accuracy against feasibility. A very simple model can be applied to a giant molecular system, but the results will be uselessly inaccurate. As noted, a very accurate model, due to its complexity, may only be feasible for systems of up to 15 electrons. However, when scientists are studying molecular systems in a field such as nanotechnology, they are interested in systems with at least a few hundred electrons.

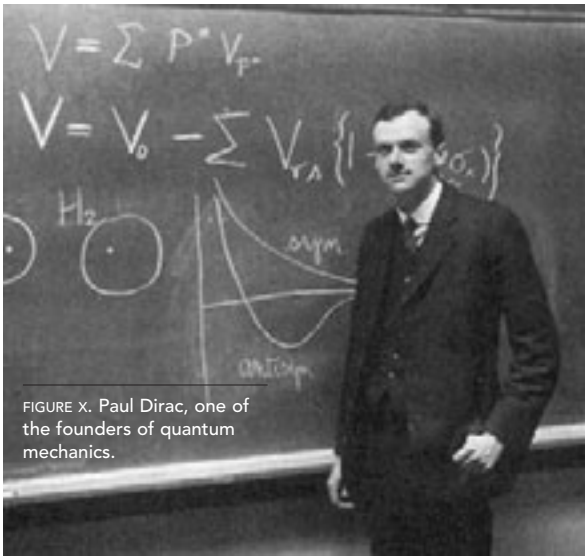


FIGURE X. Paul Dirac, one of the founders of quantum mechanics.

Realizing that a brute-force approach would not succeed, the Advanced Methods for Electronic Structure: Local Coupled Cluster Theory project was designed to develop new methods which strike novel compromises between accuracy and feasibility. The goal was to extend coupled cluster electronic structure theory to larger molecules. This was achieved by developing both new theory and new high-performance algorithms. The resulting method scales much better (at the 3rd power) than the old codes (to the 6th power), and can therefore be

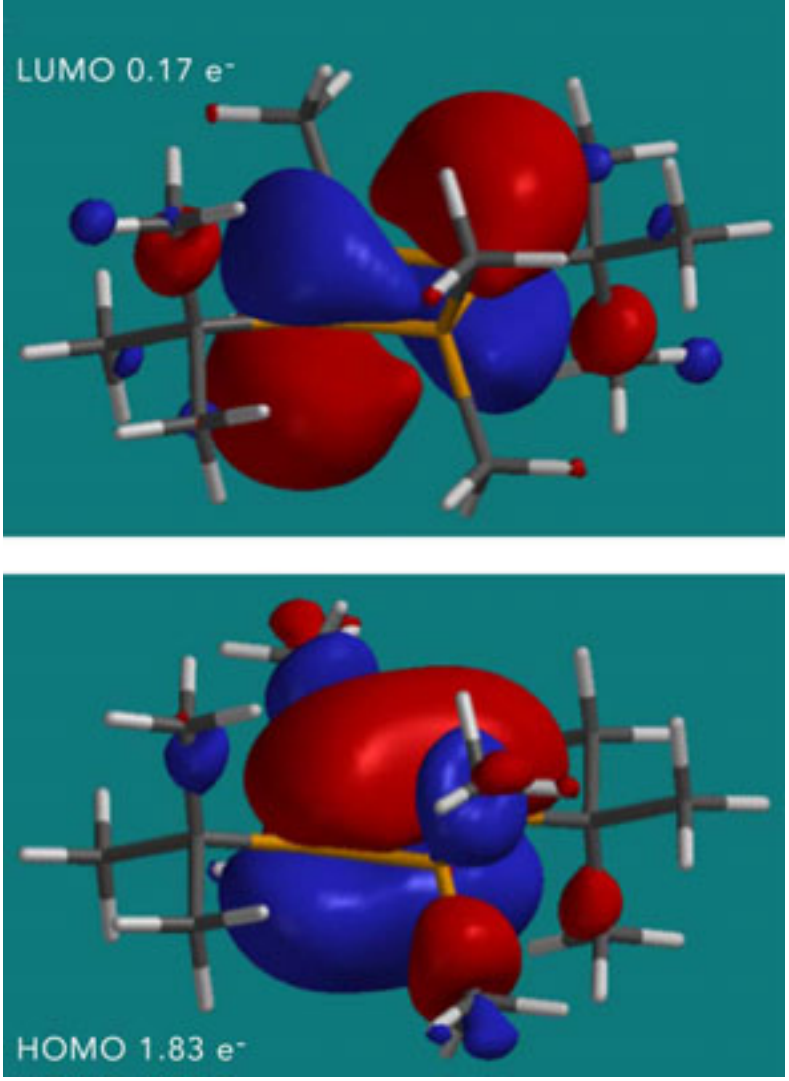


Figure 1. Graphical representation of the highest occupied molecular orbital (HOMO) and the lowest unoccupied level (LUMO) for the boron-phosphorus material. Instead of being fully empty, the LUMO contains 0.17 electrons, corresponding to 17 percent broken bond character.

applied to much larger molecules using existing supercomputers or even commodity computers.

One advantage the new method has over older methods is that it can be applied to systems where the electrons are highly correlated. In other words, the motions of the two electrons are closely tied to each other, much like two ballroom dancers or figure skaters who go through their motions almost like a single unit. Such a condition is mathematically much harder to describe than systems with weaker correlation, which can be imagined as two friends dancing separately at a rock concert. Being able to treat highly correlated electrons reliably allows scientists to study interesting molecules which would otherwise be difficult.

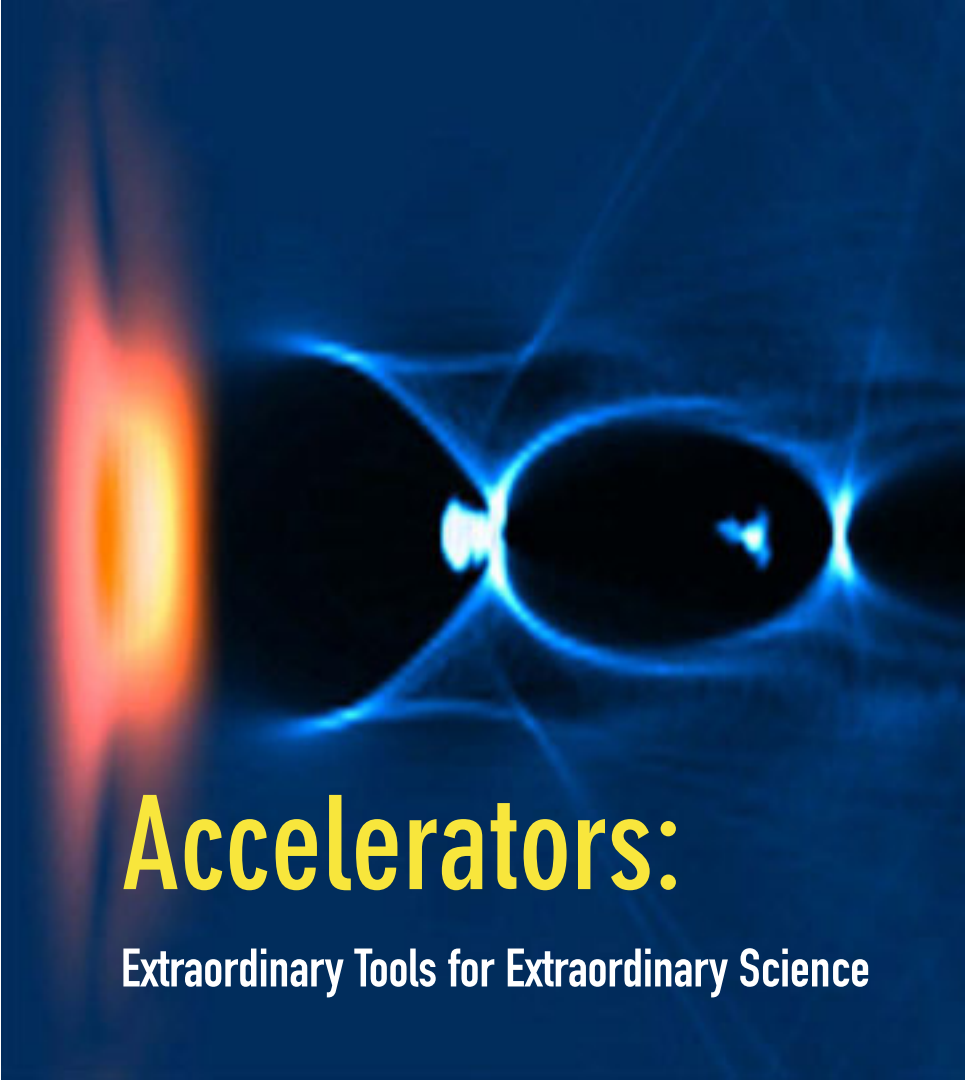
In particular, scientists have long been interested in studying molecules in which the chemical bonds are breaking, as opposed to the more common states where the molecule is either stable, with the bonds intact, or unstable, in which the bonds are broken. In bond-breaking, the electrons are strongly correlated. Scientists are interested in studying molecules as they are on their way to breaking into fragments because this may give insights that allow the design of useful materials in areas ranging from molecular electronics and spintronics to self-assembly of functional nanostructures.

The project team studied a boron-phosphorus based material that caused excitement when it was reported as the first indefinitely stable singlet diradical with the characteristics of broken bonds. The species was found computationally to have around 17 percent broken bond character, rather than the much higher fraction believed by experimentalists. This explained the stability of the material, and the origin of the 17 percent result could be understood from the role of neighboring groups, which shows the ability to tune the reactivity of the molecule by chemical design.

Project leader Martin Head-Gordon notes that the algorithms are currently not suitable for all problems, but that the team is looking to develop them into general purpose codes, and is working on improved successors. He predicts that the project's work will make its way into the mainstream within five years, bringing new computational chemistry capabilities to many of the 40,000 chemists who use such applications. Already, project members are getting inquiries from experimental chemists asking if they can use their codes to study specific molecules.

This has led to collaborations investigating the diradical character of what may be the world's longest carbon-carbon bonds as well as work in progress on triple bonds between heavier elements such as tin and germanium. Chemists are interested in whether these heavy elements can form triple bonds the way carbon does. Initial results indicate they do, but the behavior of the resulting molecules is very different.

Computation plays a key part in interpreting what experimentalists find and also in predicting what their experiments will produce, according to Head-Gordon, who has a joint appointment as a chemistry professor at the University of California, Berkeley, and DOE's Lawrence Berkeley National Laboratory. "High performance computing, together with new theory and algorithms, allows us to push the frontiers of chemistry and go where previous generations of chemists have not been able to go," Head-Gordon said.



Accelerators:

Extraordinary Tools for Extraordinary Science

Particle accelerators are some of the most powerful experimental tools available for basic science, providing researchers with insight into the basic building blocks of matter and enabling some of the most remarkable discoveries of the 20th century. They have led to substantial advances in applied science and technology, such as nuclear medicine, and are being studied for potential application to problems related to energy and the environment.

Given the importance of particle accelerators to the United States' scientific, industrial and economic competitiveness, bringing the most advanced high performance computing tools to bear on accelerator design, optimization and operation is in the national interest.

Within the DOE Office of Science, particle accelerators have enabled remarkable scientific discoveries and important technological advances that span several programs. In the High Energy Physics and Nuclear Physics programs, experiments associated with high-energy accelerators have led to important discoveries about elementary particles and the fundamental forces of nature, quark dynamics, and nuclear structure. In the Basic Energy Sciences and the Biological and Environmental Research programs, experiments with synchrotron light sources and spallation neutron sources have been crucial to advances in the materials, chemical and biological sciences. In the Fusion Energy Sciences program, great strides have been made in developing heavy-ion particle accelerators as drivers for high energy density physics research and ultimately inertial fusion energy. The importance of accelerators to the Office of Science mission is evident from an examination of the DOE "Facilities for the Future of Science: A Twenty-Year Outlook." Of the 28 facilities listed, 14 involve new or upgraded accelerator facilities.

The SciDAC Accelerator Science and Technology (AST) modeling project was a national research and development effort aimed at establishing a comprehensive terascale simulation environment needed to solve the most challenging problems in 21st century accelerator science and technology. The AST project had three focus areas: computational beam dynamics, computational electromagnetics, and modeling advanced accelerator concepts. The tools developed under this program are now being used by accelerator physicists and engineers across the country to solve the most challenging problems in accelerator design, analysis, and optimization. The following examples of scientific and engineering accomplishments achieved

by the AST project illustrate how the project software is already improving these extraordinary tools for extraordinary science.

Driving Discovery in Existing Accelerators

DOE operates some of the world's most productive particle accelerators, and one component of the AST project focused on developing scientific codes to help researchers get even more science out of these facilities.

As part of the SciDAC Accelerator Science and Technology project, the Fermilab Computational Accelerator Physics group has developed the Synergia framework. Integrating and extending existing accelerator physics codes in combination with new codes developed by the group, Synergia is designed to be a general-purpose framework with an interface that is accessible to accelerator physicists who are not experts in simulation.

In recent years, accurate modeling of beam dynamics in high-current, low energy proton synchrotrons has become necessary because of new machines under consideration for future applications, such as the High Energy Physics neutrino program, and the need to optimize the performance of existing machines, such as the Spallation Neutron Source and the Fermilab Booster. These machines are characterized by high currents and require excellent control of beam losses. A common problem in accelerators is that the particles can oscillate from the single beam, creating what is known as a "halo," which slows and weakens the particle beam. Understanding how the magnetic fields used to guide the beams can lead to this halo formation (known as a space-charge effect) is an essential component of their modeling.

Several computer simulations of space-charge effects in circular accelerators using particle-in-cell techniques have been developed. Synergia is a package for state-of-the-art simulation of linear and circular accelerators with a fully three-dimensional treatment of space charge. Space-charge calculations are computationally intensive, typically requiring the use of parallel computers.

Synergia was designed to be distributable to the particle accelerator community. Since compiling hybrid code can be a complicated task which is further complicated by the diverse set of existing parallel computing environments, Synergia includes a "build" system that allows it to be compiled and run on various platforms without requiring the user to modify the code.

When Beams Collide

While some accelerator research involves firing a beam at a stationary target, other accelerators are used to generate particle beams which are targeted to collide with each other, resulting in millions of particles flying out from the collision. High intensity, tightly focused beams result in high "luminosity," a parameter which is proportional to the number of events seen in an accelerator's detectors. But high luminosity also leads to increased beam disruption due to "beam-beam" effects, which consequently lowers the luminosity.

To better study these effects, a parallel three-dimensional, particle-in-cell code called BeamBeam3D was created to model beam-beam effects of colliding beams at high energy ring colliders. The resulting information can now be used to help accelerator operators determine the optimum parameters for colliders to maximize luminosity and hence maximize scientific output. Under SciDAC, BeamBeam3D was used to model colliding beams in several DOE accelerators including the Fermilab Tevatron, the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory, the PEP-II B-factory at Stanford Linear Accelerator Center, and the soon-to-be-operating Large Hadron Collider at CERN. In the future, BeamBeam3D is expected to be used to model beam-beam effects in the proposed International Linear Collider.

BeamBeam3D simulations of RHIC are relevant to both RHIC operations and to the future operation of the LHC (due to the similar beam-beam conditions). In regard to RHIC, the code was used to study beam-beam effects in three areas. The first are the coherent beam-beam effects. One problem is that beam-beam effects in hadron colliders, such as the one at RHIC, can create an oscillation under which the beams become unstable; this instability represents a roadblock to increasing the luminosity. Using BeamBeam3D, SciDAC researchers modeled the coherent beam-beam effects first during a collision of a single bunch of particles, then during multiple bunch collisions. In the latter case, each beam has three bunches that are coupled to three bunches in the opposite beam at four interaction points. Using the BeamBeam3D code running on high performance computers, project members were able to calculate at which point the beams would become unstable. However, the group also found that by appropriately arranging the accelerator machine lattice parameters of the two rings at RHIC and generating sufficient tune separation between the two beams, oscillation could be controlled to the extent that there is no risk of instability.

Second, using BeamBeam3D, the team studied emittance growth (a reduction in beam quality that affects the luminosity) in beams which are offset from one another. The team found that, while static offsets do not cause significant emittance growth over short time periods, the impact of offsets is much larger when they are time-modulated (due, for example, to mechanical vibrations in the final-focus magnets.) This finding provides a potential mechanism to account for the extra emittance growth observed during the machine operation.

Lastly, the team used BeamBeam3D to study long-range beam-beam effects at RHIC. Simulations performed at the energy level at which particles are injected into the accelerator showed a strong sensitivity of the long-range beam-beam effects to the machine tunes; this sensitivity was also observed in the experiments. The team subsequently modeled the long-range beam-beam effects at the higher energy levels at which the particles collide. Such simulations are providing insight and a means to numerically explore the parameter space for the future wire beam-beam compensation experiment planned at RHIC.

Shaping the Future of Accelerator Design

Although their scientific value is substantial, accelerators are very expensive and difficult to design, build and operate. As a result, the scientific community is now looking at international collaboration to develop the next generation of accelerators. One prime example is the International Linear Collider (ILC), the highest priority future project in the worldwide high energy physics community for probing into the fundamental nature of matter.

Presently, a large team of accelerator physicists and engineers from Europe, Asia and North America is working on the design of this tera-electronvolt-scale particle accelerator under a unified framework, called the Global Design Effort (GDE), to make the most of limited R&D resources. Under the AST project, modeling tools were developed and used to study the effectiveness of proposed designs and look for better solutions.

In the ILC design, two facing linear accelerators (linacs), each 20 kilometers long, hurl beams of electrons and positrons toward each other at nearly the speed of light. Each nanometer-scale size beam containing ten billion electrons or positrons is accelerated down the linac by superconducting accelerating cavities, which give them more and more energy till they meet in an intense crossfire of collisions at the interaction point. At these energies, researchers anticipate significant discoveries that will lead to a radically new understanding of what the universe is made of and how it works. The energy of the ILC beams can be adjusted to home in on elementary particle processes of interest.

A critical component of the ILC linac is the superconducting radio frequency (SRF) accelerating cavity. The design, called TESLA, was created in the early 1990s and has been the focus of more than a decade of experimental R&D effort. Recently, a new cavity design has been proposed which has a higher accelerating gradient and 20 percent less cryogenics loss over the TESLA design – an important consideration as the cavities must be cooled to extremely low temperatures (2 degrees Kelvin, or about –456 degrees Fahrenheit) to maintain superconductivity.

Accompanying intense experimental efforts at the KEK accelerator center in Japan and Jefferson Lab in Virginia, the development of this low-loss (LL) cavity has been greatly facilitated by the new parallel electromagnetic codes developed at the Stanford Linear Accelerator Center (SLAC) under the AST project. In collaboration with the SciDAC Terascale Optimal PDE Solvers Integrated Software Infrastructure Center (TOPS ISIC), the SLAC team created a nonlinear 3D parallel finite element eigensolver with which, for first time, one can directly solve for the damped dipole modes in the 3D LL cavity, complete with higher-order mode (HOM) couplers. HOM damping is essential for stable transport of "long bunch trains" of particles as they race down the ILC linacs and for preserving low emittance of particles from the beams, which can reduce their speed.

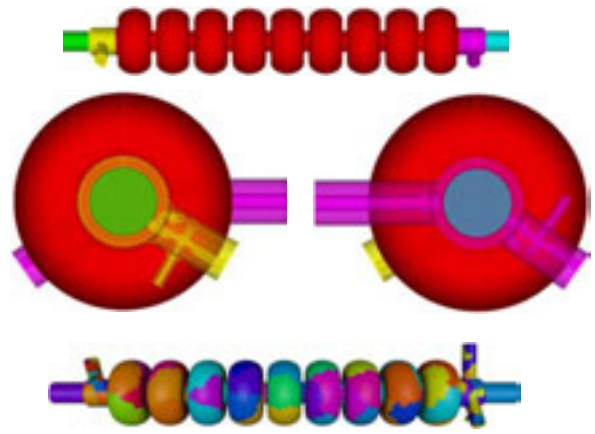


FIGURE 1. Using software developed under SciDAC, accelerator scientists developed this model of the new low-loss cavity for the proposed International Linear Collider. The different colors illustrate how various sections were modeled in parallel on multiple processors. The end perpectives show the geometry details in the couplers which could not previously be modeled because of the disparate length scales.

Previously, evaluating HOM damping in an SRF cavity took years to complete either experimentally or numerically. Today, using the tools developed under SciDAC, HOM calculations can be done in a matter of weeks with the new parallel solver running on NERSC's IBM SP3 and NCCS's Cray X1E supercomputers. In addition, the use of tetrahedral grid and higher order basis functions has enabled solutions in the complex cavity geometry to be obtained with unprecedented accuracy. As a result, costly and time-consuming prototyping by the trial-and-error approach is avoided as the LL cavity can be computationally designed as close to optimal as possible.

Advanced Accelerators: Smaller, Faster, Futuristic

DOE is also looking at future-generation accelerators, in which lasers and plasmas would be used instead of magnets to accelerate particles, which could result in accelera-

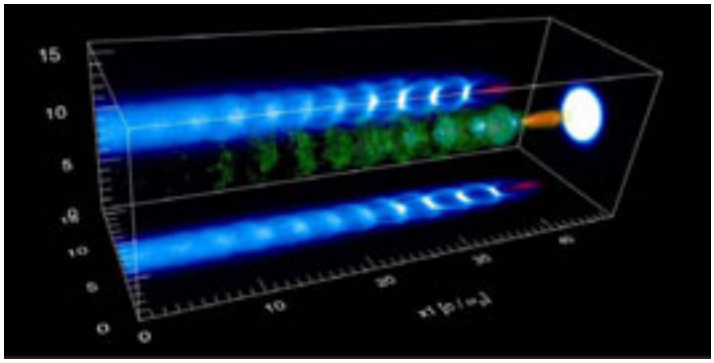


FIGURE 2. Results from a 3D OSIRIS simulation, performed at NERSC, of a beam with 2×10^{10} particles, $\sigma_r = 20$ μm and $\sigma_z = 63$ μm, propagating through a lithium gas cell of density $n_0 = 5.143 \times 10^{16}$ cm^{-3}. The simulation box was 512 × 128 × 128 grid cells wide, and the simulation was run for 3100 time steps. This 3D plot of the electron density shows the ionization electrons and wakefield as well as the drive electron bunch. Both isosurfaces and projections of this data are shown: the drive beam in red-orange-yellow colors, and background electrons in blue-cyan-green colors. (Image: R. A. Fonseca and L. O. Silva, Instituto Superior Técnico, Portugal; S. Deng and T. Katsouleas, USC; and F. S. Tsung and W. B. Mori, UCLA)

tors with 1,000 times the performance of current technology. The challenge is to control these high-gradient systems and then to string them together. Such technologies would enable the development of ultra-compact accelerators, which would be measured in meters, not kilometers. However, experiments to date have yielded only very short (only a few hundred millionths of a meter) beams of relatively poor quality, with particle energies so widespread that fewer than 1 percent have enough punch for scientific applications.

One approach being explored is a plasma-wakefield accelerator, in which a drive beam – either an intense particle beam or laser pulse – is sent through a uniform plasma. This creates a space-charge wake on which a trailing beam of particles can surf. SciDAC investigators in the Accelerator Science and Technology (AST) project have developed a suite of particle-in-cell (PIC) codes to model such devices.

SciDAC support has enabled the development of four independent, high-fidelity, particle-in-cell (PIC) codes: OSIRIS (fully explicit PIC), VORPAL (fully explicit PIC plus ponderomotive guiding center), QuickPIC (quasi-static PIC plus ponderomotive guiding center), and UPIC (a framework for rapid construction of new codes such as QuickPIC). Results from these codes were included in three articles in Nature and eight in Physical Review Letters. For example, members of the SciDAC AST project have performed large-scale simulations using the codes OSIRIS and VORPAL to help interpret laser- and plasma-wakefield accelerator experiments and to gain insight into the acceleration mechanism (Figure 3).

Researchers at Lawrence Berkeley National Laboratory took a giant step toward realizing the promise of laser wakefield acceleration, by guiding and controlling extremely intense laser beams over greater distances than ever before to produce high-quality, energetic electron beams. The experimental results were analyzed by running the VORPAL plasma simulation code, developed with SciDAC support, on supercomputers at DOE's NERSC. This allowed scientists to see details of the evolution of the experiment, including the laser pulse breakup and the injection of particles into the laser-plasma accelerator. This allows them to understand how the injection and acceleration occur in detail so that the experiment's designers can figure out how to optimize the process.

The results of the experiment and simulations were published as the cover article in the Sept. 30, 2004 issue of Nature.

Great progress has also been made in the development of reduced description models for laser/plasma simulation. One such example, QuickPIC, has been shown for some problems to provide answers as accurate as OSIRIS but with two to three orders of magnitude less computation time. Before the SciDAC effort, a full-scale simulation of a 1 TeV afterburner would have required 5 million node hours on a supercomputer (and thus was not done); after SciDAC, using QuickPIC, the simulation was done in 5,000 node hours on a cluster system.

FIGURE 3. SciDAC codes were used to analyze the experiments in two of three featured articles on compact particle accelerators in the September 30, 2004 issue of Nature.

Lattice QCD

Improved Formulations, Algorithms and Computers Result in Accurate Predictions of Strong Interaction Physics

The long-term goals of high energy and nuclear physicists are to identify the fundamental building blocks of matter and to determine the interactions among them that give rise to the physical world we observe. Major progress towards these goals has been made through the development of the Standard Model of high energy physics. The Standard Model consists of two quantum field theories: the Weinberg-Salam Theory of the electromagnetic and weak interactions, and quantum chromodynamics (QCD), the theory of the strong interactions.

The Standard Model has been enormously successful in explaining a wealth of data produced in accelerator and cosmic ray experiments over the past twenty-five years. However, our knowledge of the Standard Model is incomplete because it has been difficult to extract many of the most interesting predictions of QCD, those that depend on the strong coupling domain of the theory. The only way to extract these predictions from first principles and with controlled errors is through large-scale numerical simulations. These simulations are needed to obtain a quantitative understanding of the physical phenomena controlled by the strong interactions, to determine a number of the basic parameters of the Standard Model, and to make precise tests of the Standard Model's range of validity.

Despite the many successes of the Standard Model, it is believed that to understand physics at the shortest distances or highest energies, a more general theory, which unifies all four of the fundamental forces of nature, will be required. However, to determine where the Standard Model breaks down and new physics is required, one must first know what the Standard Model predicts.

Numerical simulations of QCD address problems that are at the heart of the Department of Energy's large experimental programs in high energy and nuclear physics. Among the major goals are (1) to calculate the effects of strong interactions on weak interaction processes to an accuracy needed to make precise tests of the Standard Model; (2) to determine the properties of strongly interacting matter under extreme conditions, such as those that existed in the very early development of the universe and are created today in relativistic heavy ion collisions; and (3) to calculate the masses of strongly interacting particles and obtain a quantitative understanding of their internal structure.

According to QCD, the funda-

mental building blocks of strongly interacting matter are quarks. Interactions among quarks are mediated by gluons, in a manner analogous to the way photons mediate the electromagnetic interactions. QCD interactions are so strong that one does not directly observe quarks and gluons under ordinary laboratory conditions. Instead, one observes strongly interacting particles, such as protons and neutrons, which are bound states of quarks and gluons. QCD was initially formulated in the four-dimensional space-time continuum; however, to carry out numerical simulations, one must reformulate the theory on a discrete four-dimensional lattice–hence the name *lattice QCD.*

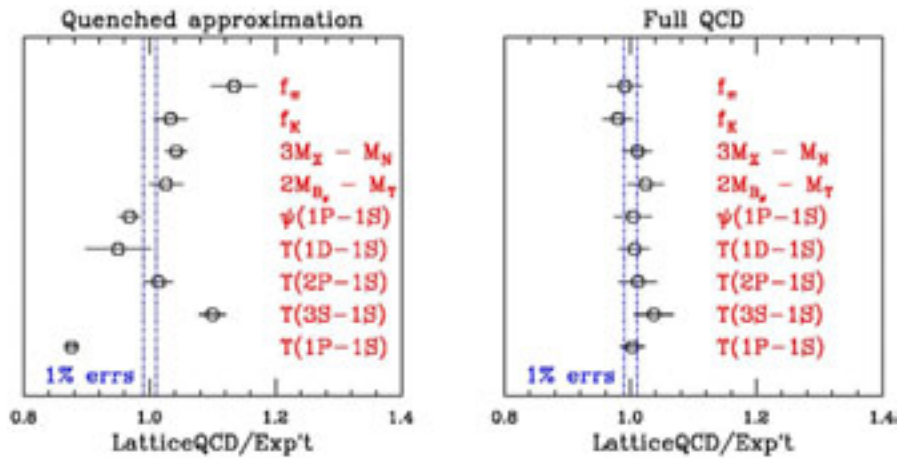


FIGURE 1. The ratio of several quantities calculated in lattice QCD to their experimental values. The panel on the left shows results from the quenched approximation, and that on the right from full QCD.

Major progress has been made in the numerical study of QCD during the course of the SciDAC program through the introduction of improved formulations of QCD on the lattice, coupled with improved algorithms and major advances in the capabilities of high performance computers. These developments have allowed physicists to fully include the effects arising from the polarization of the QCD ground state due to the creation and annihilation of quark-antiquark pairs.

The inclusion of vacuum polarization effects has been the greatest challenge to performing accurate numerical calculations of QCD. Their importance is illustrated in Figure 1, where lattice QCD calculations of the masses of a number of strongly interacting particles, and the decay constants of the π and K mesons, are compared with their experimental values. In each case, agreement with experiment was found within statistical and systematic errors of 3% or less when vacuum polarizations were included (right panel), but this was not the case when the uncontrolled approximation of ignoring vacuum polarization was made (left panel). This work was described in a "News and Views" article in Nature, as well as in a "News Focus" article in Science. Within the high energy physics community, it has been featured in Fermi News Today, Physics Today, and in a cover article in the CERN Courier.

A number of other important validations of lattice QCD methods have also been enabled by the SciDAC Program. They include the determination of the strong interaction coupling constant in agreement with but with somewhat smaller errors than the world average from a number of different experimental determinations; the determination of the nucleon axial charge, which governs the β decay of a free neutron into a proton, electron, and neutrino; and the calculation of the Cabibbo-Kobayashi-Maskawa (CKM) matrix element V_{us} to an accuracy comparable with experiment. (The CKM matrix describes how quarks couple to the weak interactions; its elements are fundamental parameters of the Standard Model.)

During the course of the SciDAC Program, the lattice QCD community moved from the validation of techniques, through the calculation of quantities that are well known experimentally, to the successful prediction of quantities that had not yet been measured. One important example was the prediction of the mass of the B_c meson. This exotic particle, which consists of a bottom quark and a charmed anti-quark, was first observed in 1998, but its mass was only poorly measured. With the aid of SciDAC-funded prototype clusters at Fermilab, the mass of the B_c meson was calculated to be 6304 ± 20 MeV, a dramatic improvement in accuracy over previous lattice calculations. Soon after this result was made public, the CDF experiment at Fermilab's Tevatron finished a new, precise measurement of the mass: 6287 ± 5 MeV, confirming the prediction from lattice QCD. The fine agreement was covered in the New Scientist, The Scotsman newspaper, and a "News and Views" article in Nature. The success of the lattice calculation was named one of the top physics stories of 2005 by Physics News Update, which described it as "the best-yet prediction of hadron masses using lattice QCD."

One of the major objectives of the field of lattice QCD is to determine the decay properties of pseudoscalar mesons with one light and one heavy quark. Strong interaction effects in leptonic decays are characterized by decay constants, while in semileptonic decays they are characterized by various form factors. The decay constants and form factors for B and B_s mesons, which contain heavy b quarks, play a critical role in

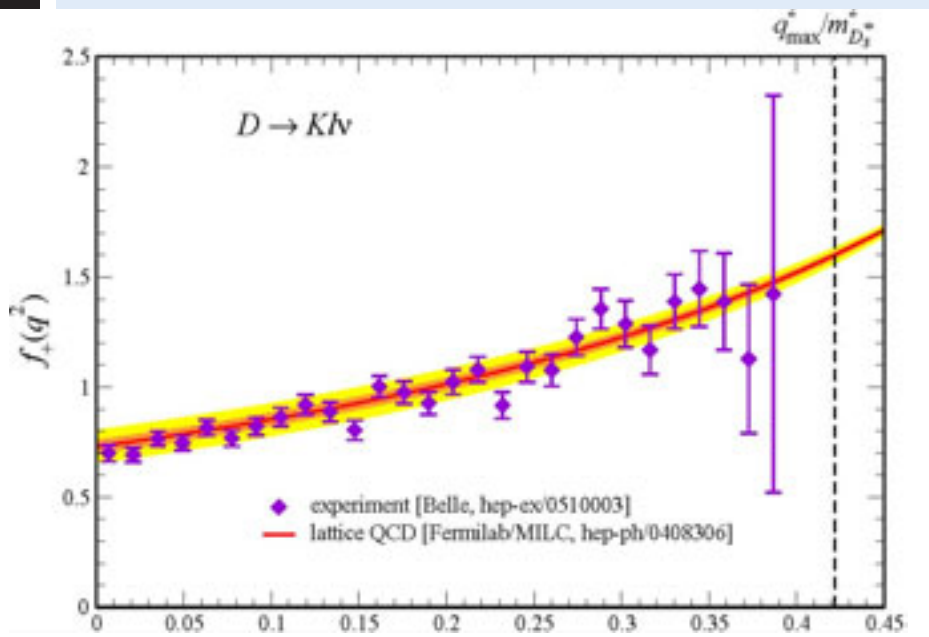


FIGURE 2. The semileptonic form factor $f+(q^2)$ for the decay of a D meson into a K meson, a lepton, and a neutrino, as a function of the momentum transfer to the leptons q^2. The orange curve is the lattice result, and the blue points are the experimental results of the Belle Collaboration.

tests of the Standard Model that are currently a major focus of the experimental program in high energy physics. These quantities are very difficult to measure experimentally, so accurate lattice calculations of them would be of great importance. On the other hand, the decay constants and form factors of D and D_s mesons, which contain heavy c quarks, are being measured to high accuracy by the CLEO-c Collaboration. Since the lattice techniques for studying mesons with c and b quarks are identical, these experiments provide an excellent opportunity to validate the lattice approach being used in the study of D and B decays.

The first lattice QCD results for the leptonic decay constants of the D and D_s mesons that fully took into account vacuum polarization effects were announced in June 2005. Within a few days of these results being made public, the CLEO-c Collaboration announced its experimental result for the decay constant of the D meson; and in April 2006 the BaBar Collaboration announced its determination of the decay constant of the D_s meson. In both cases the experiments confirmed the lattice QCD calculations with comparable errors. The lattice and experimental results for the decay of the D meson were the subjects of cover articles in the CERN Courier and the New Scientist.

Finally, the form factors that characterize the decay of a D meson into a K meson and leptons were predicted with lattice QCD in work that was also enabled by the SciDAC Program. The results were subsequently confirmed in experiments by the Focus and Belle collaborations. The lattice results are compared with experimental ones from Belle in Figure 2. The excellent agreement between theory and experiment provides one more piece of evidence that lattice QCD calculations are able to make accurate predictions of strong interaction physics. This work too was featured in Fermi News Today.

Scientific Challenge Codes: Designing Scientific Software for Next-Generation Supercomputers

For more than 40 years, the power of computer processors has doubled about every 18 months, following a pattern known as Moore's Law. This constant increase has resulted in desktop computers which today are more powerful than the supercomputers of yesteryear. Today's supercomputers, at the same time, offer computing power which enables researchers to develop increasingly complex and accurate simulations to address the most challenging scientific problems. However, the software applications for studying these problems have not kept pace with the advances in computational hardware.

Throughout the Office of Science research program are major scientific challenges that can best be addressed through advances in scientific supercomputing. These challenges including designing materials with selected properties, understanding and predicting global climate change, understanding and controlling plasma turbulence for fusion energy, designing new particle accelerators, and exploring basic questions in astrophysics.

A key component of the SciDAC program is the development of scientific challenge codes – new applications aimed at addressing key research areas and designed to take advantage of the capabilities of the most powerful supercomputers, and to run as efficiently as possible to make the most effective use of those systems.

This is a daunting problem. Current advances in computing technology are typicaly driven by market forces in the commercial sector, resulting in systems designed for commerce, not scientific computing. Harnessing commercial computing technology for scientific research poses problems unlike those encountered in previous supercomputers, both in magnitude as well as in kind. This problem will only be solved by increased investments in computer software – in research and development on scientific simulation codes as well as on the mathematical and computing systems software that underlie these codes.

In the following pages, descriptions of many of the software projects will illustrate how SciDAC has supported software development to benefit the offices of Basic Energy Research, Biological and Environmental Research, Fusion Energy Sciences and High Energy and Nuclear Physics.

Basic Energy Sciences: Understanding Energy at the Atomic Level

As one of the world's leading sponsors of basic scientific research, the Department of Energy has long supported investigations into how atoms interact, how they form molecules and how groups of atoms and molecules react with one another. Understanding the forces at work among the most basic building blocks of matter can provide greater insight into how energy is released, how waste products are generated during chemical processes and how new materials can be developed.

Within the Office of Science, the Basic Energy Sciences (BES) program supports such fundamental research in materials sciences and engineering, chemistry, geosciences and molecular biosciences. Basic research supported by the BES program touches virtually every aspect of energy resources, production, conversion, efficiency, and waste mitigation. Under the SciDAC program, a number of projects were funded to support computational chemistry.

Research in chemistry leads to advances such as efficient combustion systems with reduced emissions of pollutants, new processes for converting solar energy, improved catalysts for the producing fuels and chemicals and better methods for

environmental remediation and waste management.

Over the past 50 years, molecular theory and modeling have advanced from merely helping explain the properties of molecules to the point where they provide exact predictive tools for describing the chemical reactions of three- and four-atom systems, the starting point for many of these chemical processes. This is increasingly important as researchers seek to understand more complex molecules and processes such as combustion, which involves complex interactions of chemistry with fluid dynamics.

The advances in computational chemistry in recent years in providing accurate descriptions of increasingly complex systems have come as much from improvements in theory and software as from improved computational hardware. However, the computational requirements often outweigh the scientific gains. For example, electronic structure theory provides the framework for modeling complex molecular-level systems (from atoms to thousands of atoms) with increasing accuracy. But accurate electronic structure theories have computational costs that rise with the 6th power (or higher) of molecular size, so that 10 times the computing resources translates into treating a system less than 1.5 times bigger. Predictive modeling of such processes is currently beyond the capabilities of existing computational resources and computational methods.

Under the SciDAC program, BES supported a number of projects aimed at developing computational approaches to solving problems in the modeling of chemical processes that exceed current computational capabilities. These projects were selected to increase the accuracy of models, increase the size of systems which could be simulated and expand the capabilities of key applications already being used in the research community.

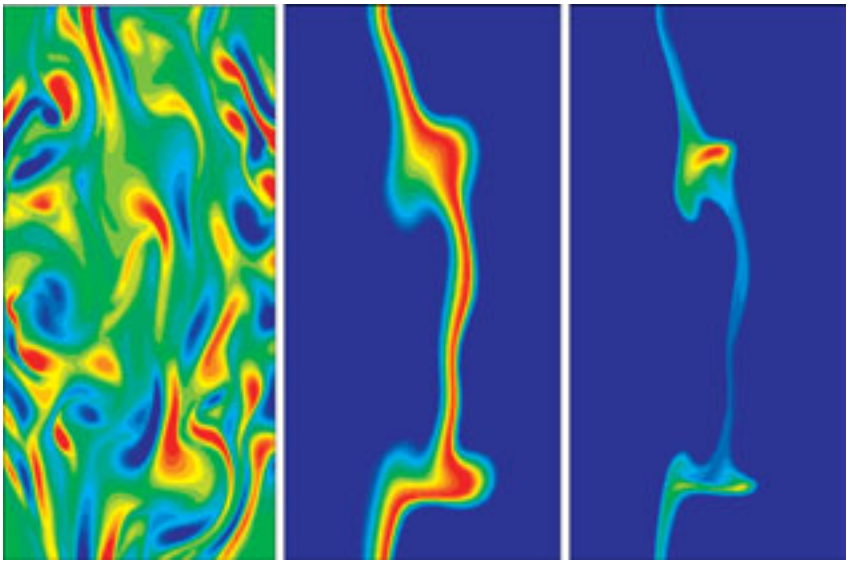


FIGURE 1: Simulations of turbulent nonpremixed ethylene-air flames reveal detailed structure of dynamics of the soot formation process. Shown from left to right are instantaneous images of the vorticity, temperature, and soot volume fraction.

Two of the projects focused on improving computational modeling of combustion, which is key to 80 percent of the energy production in the United States. Developing new methods to make combustion more efficient and cleaner will benefit the economy, the environment and the quality of life. With such a prominent role in energy production and use, combustion has long been an important research focus for the DOE.

But fully understanding combustion is an extremely complex problem involving turbulent flows, many chemical species and a continuing series of interdependent chemical processes and reactions. As computers have become more powerful, more detailed combustion simulations can be created to help scientists better understand the process.

The Terascale High-Fidelity Simulations of Turbulent Combustion with Detailed Chemistry project is a multi-university collaborative effort to develop a high-fidelity turbulent reacting flow simulation capability that can take advantage of the most powerful supercomputers available. The approach is based on direct numerical simulation (DNS) to enable the highest accuracy and allow scientists to study the fine-scale physics found in turbulent reacting flows.

Under SciDAC, the simulation code named S3D has been enhanced with many new numerical algorithms and physical models to provide predictive capabilities for many of the detailed processes which occur during combustion, including thermal radiation, soot dynamics, spray injection and evaporation, and flame-wall interaction. The S3D code was used to perform detailed three-dimensional combustion simulations of flames in which fuel and oxygen are not premixed. This research could have applications in such areas as jet aircraft engines, where fuel and oxidizers are not premixed for safety reasons, and in direct-injection internal combustion engines. Under certain conditions, this type of combustion can suddenly and unexpectedly become extinguished, and this project is expected to lead to a better understanding of this problem, as well as re-ignition of extinguished flames. The team demonstrated the advanced DNS capability by undertaking several laboratory-scale simulations to high-

light fundamental aspects of turbulence-chemistry interaction occurring in many practical combustion systems.

Principal Investigators: Hong G. Im, University of Michigan; Arnaud Trouvé, University of Maryland; Christopher J. Rutland, University of Wisconsin; and Jacqueline H. Chen, Sandia National Laboratories

The Computational Facility for Reacting Flow Science project is aimed at advancing the state of the art in the understanding and prediction of chemical reaction processes, such as combustion, and their interactions with fluid flow. Such detailed reacting flow computations are computationally intensive, yet they provide information that is necessary for the understanding and prediction of turbulent combustion. The project's approach towards achieving this goal includes two broad focus areas. The first involves developing high-accuracy adaptive mesh refinement (AMR) algorithms and implementing them in a flexible software toolkit for reacting flow computations. The second involves the development of advanced chemical analysis algorithms and software that enable both the extraction of enhanced physical understanding from reacting flow computations, and the development of chemical models of reduced complexity. The overall construction is being implemented in the context of the common component architecture (CCA) framework. The assembled software will be applied to targeted reacting flow problems, in two and three dimensions, and validated with respect to reacting flow databases at the Combustion Research Facility of Sandia National Laboratories.

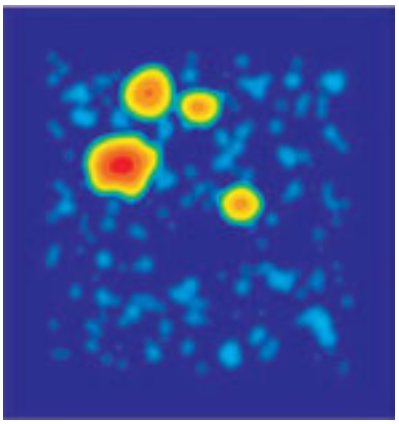


FIGURE 2. Reaction-diffusion high-order AMR computations of the propagation of random premixed hydrogen-oxygen ignition kernels in two dimensions. The temperature field is shown, indicating cold reactants (blue) and hot combustion products (red), separated by the propagating flame fronts.

Principal Investigator: Habib Najm, Sandia National Laboratories

Another set of projects focused on improving applications for modeling electronic structure. Electronic structure calculations, followed by dynamical and other types of molecular simulations, are recognized as a cornerstone for the understanding and successful modeling of chemical processes and properties that are relevant to combustion, catalysis, photochemistry, and photobiology.

The **Advanced Methods for Electronic Structure** project advanced the capabilities of quantum chemical methods to describe efficiently and with controllable accuracy the electronic structure, statistical mechanics, and dynamics of atoms, molecules and clusters. The project, which had goals of improving the speed, scalability and accuracy of electronic structure applications, had two thrusts.

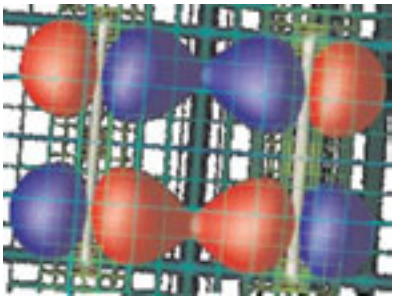


FIGURE 3. Molecular orbital of the benzene dimer with the adaptive grid and an isosurface.

(1) The **Multiresolution Quantum Chemistry – Guaranteed Precision and Speed** component worked to increase the accuracy of chemistry codes as they are scaled up to run on larger systems, while also reducing the amount of processing time needed to run the calclulations. Additionally, computational chemistry is expected to benefit from the resulting computational framework that is substantially simpler than conventional atomic orbital methods, that has robust guarantees of both speed and precision, and that is applicable to large systems. In contrast, current conventional methods are severely limited in both the attainable precision and size of system that may be studied. The project achieved its goals for effective one-electron theories and is studying many-body theories. The electronic structure methods should be valuable in many disciplines, and the underlying numerical methods are broadly applicable.

Principal Investigator: Robert Harrison, Oak Ridge National Laboratory

(2) The component to develop **Advanced Methods for Electronic Structure: Local Coupled Cluster Theory** was designed to extend coupled cluster (CC) electronic structure theory to larger molecules ("coupled cluster" is a numerical technique used for describing many-body systems). This method was achieved by developing novel "fast" coupled cluster algorithms that are much more scalable with respect to system size to more fully realize the potential of high performance computing for treating larger molecular systems. CC methods are well established as the wave-function-based electronic structure method of choice. However, even the simplest CC method, incorporating just correlations between pairs of electrons (double substitutions), still requires computational costs that

scale with the 6th power of the size of the molecule. This research focused on defining new and powerful "local correlation" models that reduce scaling of coupled cluster calculations, and developing effective algorithms for their implementation.

Principal Investigator: Martin Head-Gordon, Lawrence Berkeley National Laboratory

The project for **Advancing Multi-Reference Methods in Electronic Structure Theory** researched and developed new models for investigating detailed mechanisms of chemical reactions for complex systems, including biomolecular processes, such as the interaction of protein molecules. Specifically, the project worked on the development of highly scalable electronic structure codes that are capable of predicting potential energy surfaces of very high accuracy, which is important since potential energy surfaces determine how atoms and chemical bonds rearrange during chemical reactions. The ability to study extended systems containing tens to thousands of atoms with reasonable accuracy is of paramount importance. The development of methods to adequately treat such systems requires highly scalable, highly correlated electronic structure methods interfaced with classical methods and mesoscale codes.

Principal Investigator: Mark S. Gordon, Ames Laboratory

The **Advanced Software for the Calculation of Thermochemistry, Kinetics and Dynamics** project consisted of two integrated programs to develop both scalable kinetics/dynamics software and infrastructure software. The overall thrust is to develop software to efficiently provide reliable thermochemistry (heat-related chemical reactions), kinetics, and dynamics for large molecular systems. Kinetics/dynamics studies compute how molecules move over a potential energy surface. The first goal is to provide better thermochemistry for larger systems and improve the performance of related components in the Columbus computational chemistry software system. The second goal is to develop highly parallelized quantum dynamics and quantum kinetics software. Lastly, common component architecture techniques will be used to integrate kinetics and electronic structure software into a package that will allow users to compute kinetics information just by specifying the reactants. The infrastructure program's focus is on preconditioners (tools which improve convergence rates of certain mathematical methods) and on potential energy surface fitting schemes that reduce the number of electronic structure calculations necessary for accurate kinetics and dynamics. The infrastructure software has benefited from Integrated Software Infra-structure Centers (ISIC) support.

Principal Investigators: Albert F. Wagner (2001-03), Ron Shepard (2004-05), Argonne National Laboratory

The **Theoretical Chemical Dynamics Studies of Elementary Combustion Reactions** project involved modeling the dynamics of chemical reactions of large polyatomic molecules and radicals important in combustion research, using a combination of theories and methods. These computationally challenging studies will test the accuracy of statistical theories for predicting reaction rates, which essentially neglect dynamical effects. This research is expected help extend theoretical chemical dynamics to the treatment of complex chemical reactions of large polyatomic molecules.

Principal Investigator: Donald L. Thompson, University of Missouri

Biological and Environmental Research: Advanced Software for Studying Global Climate Change

In many fields of scientific research, scientists conduct experiments to test theories, then analyze the results, and use the information to continue refining their theories and/or experiments as they gain additional insight. In the study of global climate change, however, the "experiment" takes place day after day, year after year, century after century, with the entire planet and its atmosphere as the "laboratory." Climate change literally affects each and every person on Earth and because any measures taken to address the issue will have far-reaching social, economic and political implications, it's critical that we have confidence that the decisions being made are based on the best possible information.

Scientists have thought for more than 100 years that increasing atmospheric concentrations of carbon dioxide (CO_2) and other greenhouse-gases from human activity would cause the atmospheric layer closest to the Earth's surface to warm by several degrees. Because of the complex feedbacks within the Earth system, precisely estimating the magnitude and rate of the warming, or understanding its effects on other aspects of climate, such as precipitation, is a daunting scientific challenge. Thanks to a wealth of new observational data and advances in computing technology, current climate models are able to reproduce the global average temperature trends observed over the twentieth century and provide evidence of the effect of human activity on today's climate.

The Climate Change Research

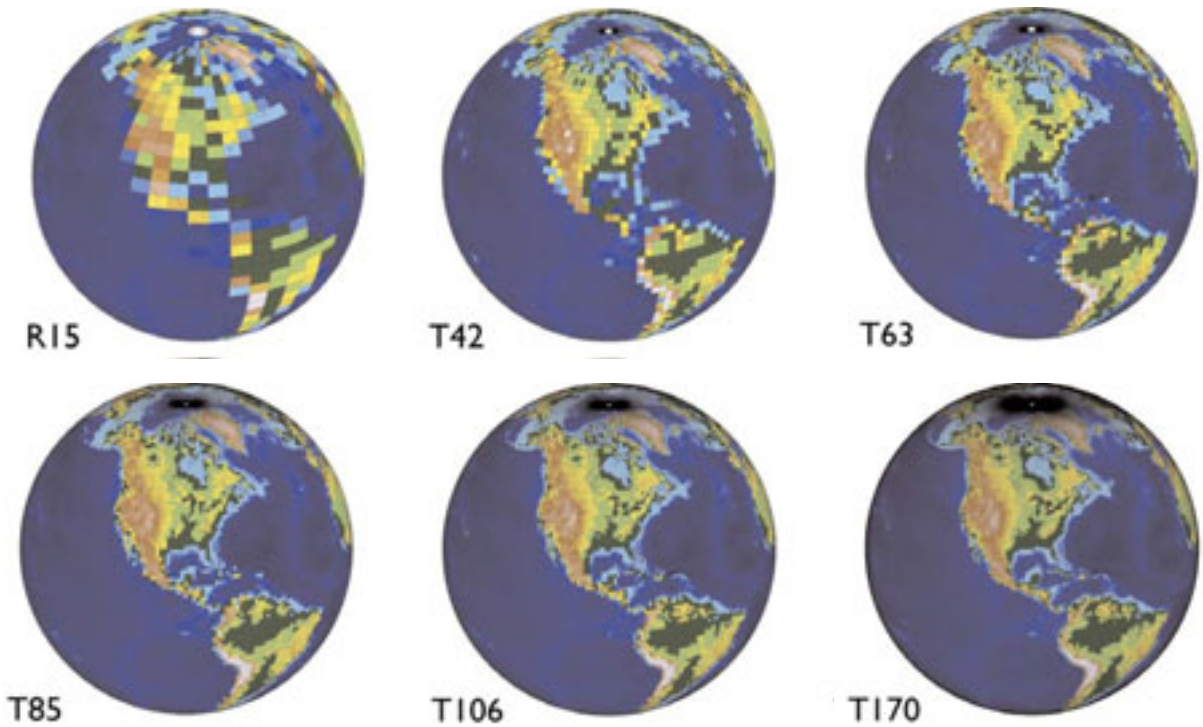


FIGURE 4. As supercomputers have become more powerful, climate researchers have developed codes with finer and finer resolution, allowing the models to incorporate more details which affect climate. The resulting climate models are more accurate.

Division in the DOE Office of Science was established "… to advance climate change science and improve climate change projections using state-of-the-science coupled climate models, on time scales of decades to centuries and space scales of regional to global."

Fortunately, the growing power and capabilities of high-performance computers are giving climate researchers more accurate tools for analyzing and predicting climate change. Climate, whether in our neighborhood, our region or continent, is determined by many factors, some local, others global. Geography, air temperature, wind patterns, ocean temperature and currents and sea ice are among the forces that shape our climate. As a result, comprehensive climate models which couple together simulations of different processes are among the most complex and sophisticated computer codes in existence. While they can simulate most of the continental-scale features of the observed climate, the models still cannot simulate, and therefore cannot predict, climate changes with the level of regional spatial accuracy desired for a complete understanding of the causes and effects of climate change.

As climate science advances and new knowledge is gained, there is a demand to incorporate even more factors into the models and to improve acknowledged shortcomings in existing models. These demands, which make the models more accurate, will unfortunately overwhelm even the most optimistic projections of computer power increases. So, a balance must be struck between the costs, benefits and tradeoffs required to allocate scarce computer and human resources to determine which improvements to include in the next generation of climate models.

Under SciDAC, teams of climate researchers worked to develop improved computational tools and techniques for studying and modeling climate change, focusing on the numerical and computational aspects of climate modeling. In particular, SciDAC funding has enabled DOE researchers to participate with NSF and NASA researchers over an extended period in the design and implementation of new climate modeling capabilities. There are three major pieces, two of which pursued research in the academic arena that was longer term and more basic.

A National Consortium to Advance Global Climate Modeling

The major SciDAC effort in climate modeling was a multi-disciplinary project to accelerate development of the Community Climate System Model (CCSM), a computer model of the Earth's climate that combines component models for

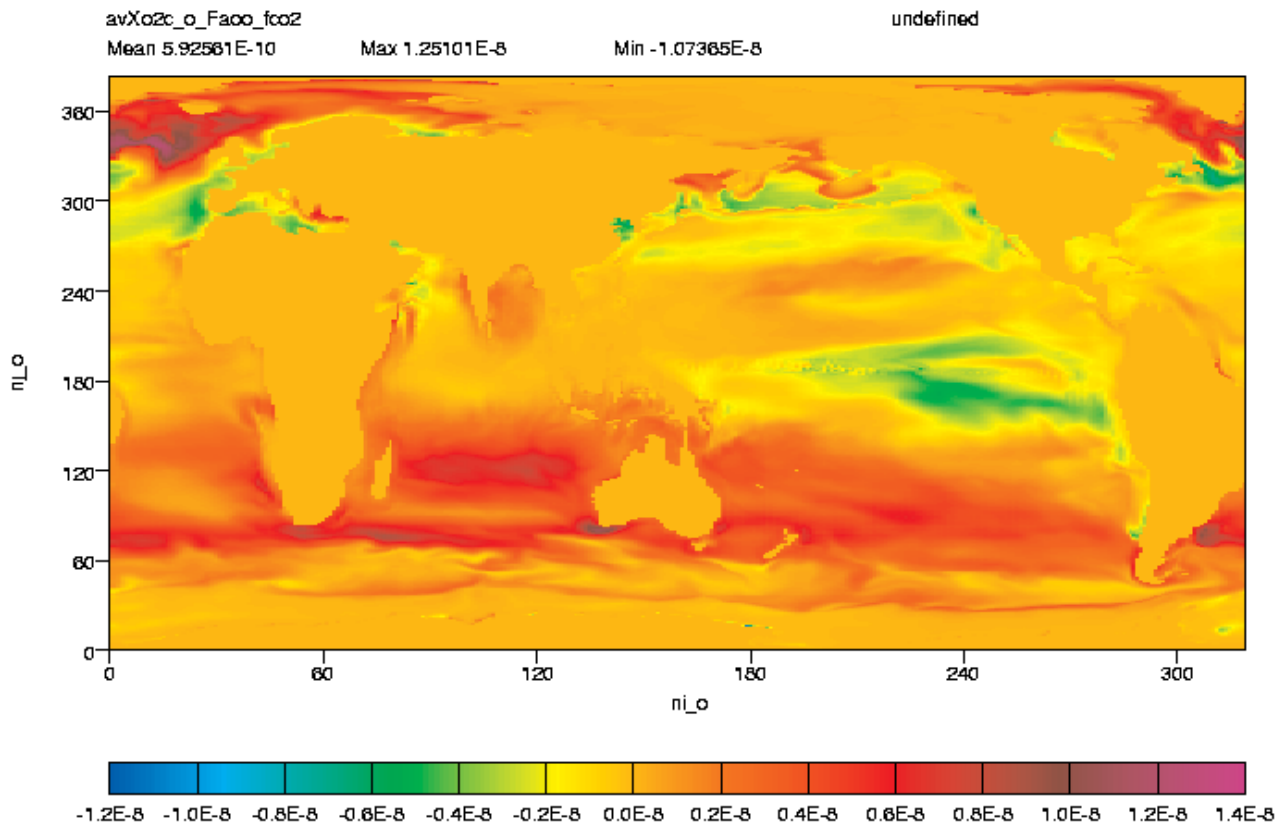


FIGURE 5. The flux of CO_2 between the ocean and the atmosphere as handled by the bigeochemical coupler. The red values show those regions where CO_2 is moving from the ocean to the atmosphere, and the yellow to blue values show where the ocean is a sink of atmospheric CO_2 and carbon is moving from the atmosphere to the ocean.

the atmosphere, ocean, land and sea ice. The CCSM is developed by researchers from NSF, DOE, NASA and NOAA laboratories, as well as universities. As one of the leading climate models in the United States, CCSM has a large user base of several hundred climate scientists. The CCSM community contributed a large number of climate change simulation results for the periodic Intergovernmental Panel on Climate Change (IPCC) climate assessment report. The **Collaborative Design and Development of the Community Climate System Model for Terascale Computers** project had two goals.

The first goal was to improve software design and engineering of the CCSM and its component models and improve performance portability across the wide variety of computer architectures required for climate assessment simulations. The second goal was to accelerate the introduction of new numerical algorithms and new physical processes within CCSM models.

Under SciDAC, a consortium of six national laboratories and researchers from the National Center for Atmospheric Research (NCAR) and NOAA worked together on a variety of improvements to the CCSM. In the early years of the five-year project, attention was focused on improving the performance and portability of CCSM on the wide variety of vector and scalar computers available to the community.

The atmosphere and ocean models were improved with the introduction of new flexible data decomposition schemes to enable tuning for each computational platform. The sea ice and land models were restructured to improve performance, particularly for vector computers, and new software was developed to improve the coupling of the four components into a fully coupled model.

These changes enabled the largest ensemble of simulations – 10,000 years worth – of any modeling group in the world for the recent IPCC assessment. These simulations were performed at relatively high resolution, generating more than 110 terabytes of climate model data, which were distributed internationally via the SciDAC-funded Earth System Grid. This important contribution to the international climate research effort was made pos-

sible by the critical software engineering work performed by the SciDAC team members on all the components of CCSM.

In addition to software expertise, the SciDAC CCSM consortium also contributed new model algorithms and new scientific capabilities. The consortium contributed to the introduction of a new finite-volume method for simulating atmospheric dynamics and developed new alternative schemes for ocean models as well.

Details of the consortium's software engineering of the CCSM were reported in articles featured in a special issue on climate modeling of the *International Journal of High Performance Computing and Applications* (Vol. 19, No. 3, 2005).

In the last years of the project, the focus of the SciDAC consortium was the development of new capabilities for simulating the carbon and sulfur cycles as part of the climate system. Until recently, most climate change scenarios specify a concentration of greenhouse gases and atmospheric aerosols. By adding the biological and chemical processes that govern the absorption and emission of greenhouse gases, better simulations of how the Earth system responds to human-caused emissions are possible (see Figure 1). A prototype carbon-climate-biogeochemistry model was assembled as a demonstration of the readiness to undertake coupled Earth system simulation at this dramatically new level of complexity.

The new model included a comprehensive atmospheric chemistry formulation as well as land and ocean ecosystem models. In this first step towards a comprehensive Earth system model, CO2 fluxes were exchanged between components (see Figure 2) and the oceanic flux of dimethyl sulfide (DMS) was used in the atmospheric model to create sulfate aerosols. These aerosols then interacted and affected the physical climate system, the oceanic carbon cycle and terrestrial ecosystems. The prototype model developed under SciDAC will form the basis for future work on a comprehensive Earth system model and help the climate community enter a new phase of climate change research.

Principal Investigators: John Drake, Oak Ridge National Laboratory, Phil Jones. Los Alamos National Laboratory

A Brand New Model

Under SciDAC, DOE's Office of Biological and Environmental Research pursued the novel concept of a five-year cooperative agreement with one or two universities to build the prototype climate model of the future. The concept was to develop a new climate model without the legacies of past approaches, which may be scientifically or computationally outdated. Only one qualified proposal was submitted, that from a group centered at Colorado State University, which is developing a model using a radically different grid design, alternative formulations for both the atmosphere and ocean components and alternative numerical methods.

The project, **A Geodesic Climate Model with Quasi-Lagrangian Vertical Coordinates,** was created to develop a new, comprehensive model of the Earth's climate system that includes model components for the atmosphere, ocean, sea-ice, and land surface, along with a model coupler to physically link the components. A multi-institutional collaboration of universities and government laboratories in an integrated program of climate science, applied mathematics and computational science, this project built upon capabilities in climate modeling, advanced mathematical research, and high-end computer architectures to provide useful projections of climate variability and change at regional to global scales. The project team developed components for modeling the atmosphere, oceans and sea ice, and a coupler component to links the physical model components. For example, the coupler computes the

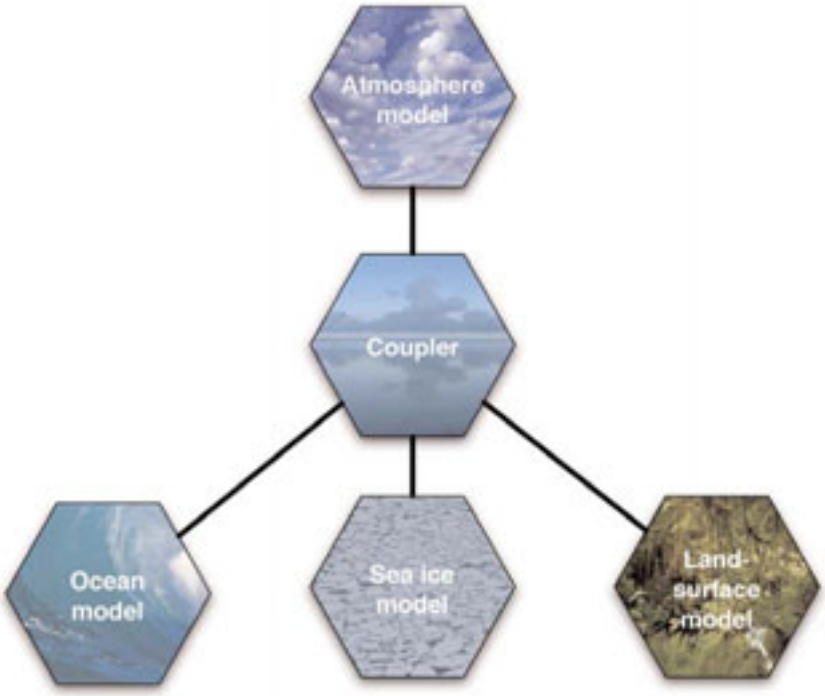


FIGURE 6. By coupling different climate modeling components, climate researchers can take advantage of advancements in the separate codes to improve overall accuracy.

latent heat flux exchanged between the ocean surface and atmosphere. This physical coupling enables the coupled system to evolve in a coherent manner. As the pieces come together the integrated system is being thoroughly tested.

Principal Investigator: David A. Randall, Colorado State University

University-Led Climate Modeling Projects

SciDAC supported two rounds of university grants to individual researchers to address the 5- to 15-year needs and opportunities to advance climate modeling. These grants supported research into new methodologies and numerical methods. It is this basic research that explores new ideas and concepts that tie climate science and computational science together as both fields advance.

A major factor in climate change between decades is the effect of winds on ocean circulation. The project on **Predictive Understanding of the Oceans: Wind-Driven Circulation on Interdecadal Time Scales** was aimed at developing and applying advanced computational and statistical methods to help climate models better predict these effects. The computational aspect of the project was aimed at developing efficient multi-level methods to simulate these ocean flows and study their dependence on physically relevant parameters. The oceanographic and climate work consists in applying these methods to study the bifurcations in the wind-driven circulation and their relevance to the flows observed at present and those that might occur in a warmer climate. Both aspects of the work are crucial for the efficient treatment of large-scale, eddy-resolving numerical simulations of the oceans and an increased understanding of climate change.

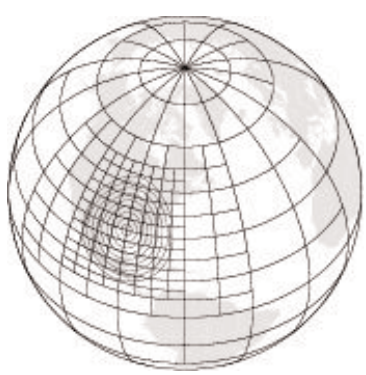


FIGURE 7. Adapted grid with block-data structure.

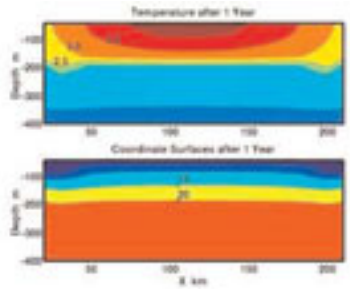


FIGURE 8. A vertical cross section from the model. (Upper panel) The penetration of the temperature field into the hybrid model. The lateral exchange of heat by the model circulation prevents a deep penetration of the imposed temperature anomalies. (Lower panel) The configuration of the hybrid coordinate surfaces. Note the coordinate surface is pushed upwards in response to surface heating at the center and downwards in response to cooling at the edges.

Principal Investigators: Michael Ghil, UCLA; and Roger Temam, Indiana University

With the advent of more powerful supercomputers and modeling applications, climate models, resolution of the globe has become increasingly precise – to the extent that some models can focus on an area as small as 10 kilometers square. While this is useful for large-scale climate conditions, understanding smaller phenomena such as tropical storms require 1-km resolution. **The Continuous Dynamic Grid Adaptation in a Global Atmospheric Model** is aimed at providing a capability to break down the larger grid structure to target areas of interest. While climate models are not expected to provide a uniform 1-km resolution within the next 15 years, this grid adaptation capability is a promising approach to providing such resolution for specific conditions.

Principal Investigators: J.M. Prusa and W.J. Gutowski, Iowa State University

While much discussion of climate change focuses on the global scale, there is also increasing demand for climate modeling on the regional or mesoscale covering areas from 50 to several hundred miles in size. The project to develop **Decadal Climate Studies with Enhanced Variable and Uniform Resolution GCMs Using Advanced Numerical Techniques** focused on using developed and evolving state-of-the-art general circulation models (GCMs) with enhanced variable and uniform resolution to run on parallel-processing terascale supercomputers. The major accomplishment of the project was completion of the international SGMIP-1 (Stretched-Grid Model Intercomparison Project, phase-1), which allows smaller regional models to be computed as part of global modeling systems. The "stretched grid" approach provides an efficient down-scaling to mesoscales over the area of interest and computes the interactions of this area with the larger model. This capability is expected to improve our understanding of climate effects on floods, droughts, and monsoons.

Collaboration with J. Côté of MSC/RPN and his group is a strong integral part of the joint effort. The companion study with the members of another SciDAC group, F. Baer and J. Tribbia, is devoted to developing a stretched-grid GCM using the advanced spectral-element technique with variable resolution, and the NCAR CAM physics.

Principal Investigator: Michael S. Fox-Rabinovitz, University of Maryland

The project for **Development of an Atmospheric Climate Model with Self-Adapting Grid and**

Physics was funded to develop adaptive grid techniques for future climate model and weather predictions. This approach will lead to new insights into small-scale and large-scale flow interactions that cannot be modeled by current uniform-grid simulations. This project will result in a climate model that self-adjusts the horizontal grid resolution and the complexity of the physics module to the atmospheric flow conditions. Using an approach called adaptive mesh refinement to model atmospheric motion will improve horizontal resolution in a limited region without requiring a fine grid resolution throughout the entire model domain. Therefore, the model domain to be resolved with higher resolution is kept at a minimum, greatly reducing computer memory and speed requirements. Several tests show that these modeling procedures are stable and accurate.

Principal Investigator: Joyce E. Penner, University of Michigan

The credibility of ocean models for climate research depends on their ability to simulate the observed state and natural variations of the oceans as indicated by actual measurements. Existing models, which can be used for simulating the long time scales of climate change of the order of centuries, still do not provide a very satisfactory treatment of key climatic processes such as water mass formation in the subpolar oceans. Ocean models based on Cartesian coordinates have been well tested and their drawbacks are well known. Models based on a moving vertical coordinate have the potential to provide a much more accurate simulation, but are not "mature'" enough at present to gain widespread acceptance in the climate modeling community. The project to develop **A Vertical Structure Module for Isopycnal Ocean Circulation Models** aimed at providing a module for representing key processes in such a model and organizing the vertical structure. The module can then be inserted in the 'dynamic core' of existing models and used by the modeling community.

Principal Investigator: Kirk Bryan, Princeton University

The advent of terascale supercomputers has advanced climate modeling by allowing the use of higher-resolution atmospheric and ocean models. However, more dramatic improvements are likely through development of improved descriptions of physical processes treated by the models, especially those that can be observationally characterized in much finer details than are conventionally included in the climate models. The project for **Improving the Processes of Land-Atmosphere Interaction in CCSM 2.0 at High Resolution** has contributed to this goal by advancing the treatment of land with much improved details in the climatically most important processes, using primarily the Community Land Model (CLM).

Principal Investigator: Robert E. Dickinson, Georgia Institute of Technology

As part of the effort to develop climate models for making reliable climate predictions, one need is for an efficient and accurate method for producing regional climate predictions and the development of computing methodology which uses the latest in computing hardware (massively parallel processing or MPP) most efficiently and economically, to produce the best prediction results with minimal expenditure of resources. To meet this goal, the **Multi-Resolution Climate Modeling** project developed a Spectral Element Atmospheric Model (SEAM), a fairly recent concept using spectral elements (a method of approximating mathematical solutions). The Earth's spherical domain is tiled with spectral elements that can be arbitrarily sized to meet local scaling requirements, allowing the model to create predictions over a range of scales on the entire global domain without user involvement in the computational process. The method also takes optimum advantage of state-of-the-art MPP by minimizing communication among elements and thereby amongst processors. This procedure has yielded dramatic speedup, making the production of multiple realizations more feasible. In addition to serving as a research and training tool, the model is expected to provide more accurate climate predictions.

Principal Investigator: Ferdinand Baer, University of Maryland

The **Decadal Variability in the Coupled Ocean-Atmosphere System** project researched the slowly changing circulations in the oceans and their influence on long-term global climate variability. There were two main themes in the project. The first concerned the decadal variability of upper ocean circulation and its role in the long period fluctuations of the coupled ocean/atmosphere system. The second was the role of mesoscale eddies – the oceanic flows on scales of 10 to 100 km – in the large-scale heat and energy budget of the ocean. The model was developed and tested on a smaller computer and will be adapted for use on larger massively parallel supercomputers.

Principal Investigator: Paola Cessi, Scripps Institution of Oceanography – University of California, San Diego

A project called **Towards the Prediction of Decadal to Multi-Century Processes in a High-Throughput Climate System Model** pursued interdisciplinary research to simulate decadal to multi-century global variability and change in an earth system model that couples climate to the terrestrial ecosystem. The primary tool will be a high-throughput climate-ecosystem model called FOAM that enables rapid turnaround on long climate runs. FOAM is used to continue the study of the mechanisms of decadal climate variability, the

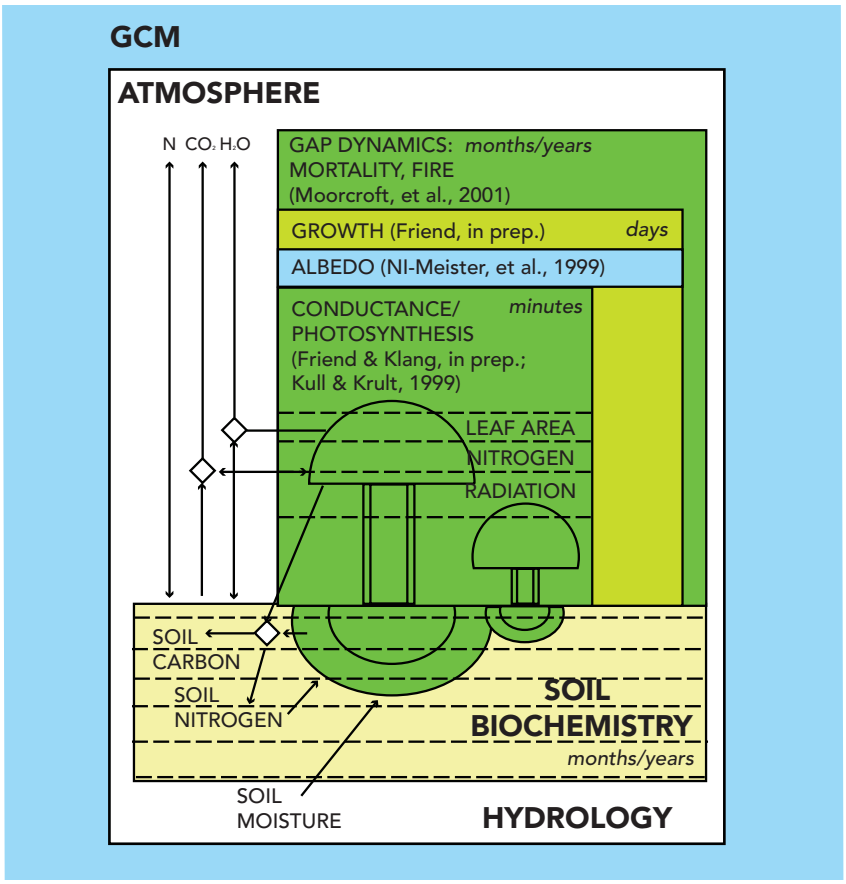


FIGURE 9. Diagram of the dynamic vegetation embedded within the atmospheric and land surface components of a GCM.

dynamics of global warming, and the interaction of climate and the land biosphere. The project also linked climate scientists with ecosystem modelers in building a fully coupled ocean-atmosphere-land biosphere model, which enabled the study of the interaction of land vegetation changes and climate changes for past, present, and future scenarios.

Principal Investigator: Zhengyu Liu, University of Wisconsin-Madison

Vegetation is an important component of the global climate system through its control of the fluxes of energy, water, carbon dioxide and nitrogen over land surfaces. The aim of the project for **Modeling Dynamic Vegetation for Decadal to Century Climate Change Studies** is to develop, evaluate, utilize and make available a model of vegetation/soil dynamics to improve the ability of general circulation models (GCMs) to make predictions of future climate change. The model is being developed by combining treatments of carbon and nitrogen fluxes, and vegetation community dynamics, as a standalone module within the NASA Goddard Institute for Space Studies GCM. This model will be a tool for answering questions about past climate and vegetation distributions, as well as for predicting global changes due to rising atmospheric CO_2 in the coming decades and century. In one scenario, in which the concentration of CO_2 in the atmosphere was doubled, the model showed that vegetation increased the uptake of CO_2 by 48 percent and that surface temperatures in some regions increased by up to 2° C due to stomatal closure.

Principal Investigator: Nancy Y. Kiang, Columbia University

Gaining a better understanding of the relationship between climate change and the transport of water vapor and chemicals in the atmosphere was the aim of the **Modeling and Analysis of the Earth's Hydrologic Cycle** project. This research addresses fundamental issues underlying the understanding and modeling of hydrologic processes, including surface evaporation, long-range transport of water, and the release of latent heating through evaporation. These processes play a central role in climate. The goals of the project are to advance climate change modeling by developing a hybrid isentropic model (in which the flow variables change gradually) for global and regional climate simulations, to advance the understanding of physical processes involving water substances and the transport of trace constituents, and to examine the limits of global and regional climate predictability.

Principal Investigator: Donald R. Johnson, University of Wisconsin – Madison

Fueling the Future: Plasma Physics and Fusion Energy Research

Plasmas, or very hot ionized gases, make up more than 99 percent of the visible universe. In fact, the earth's sun and the stars we see at night are masses of plasma burning at millions of degrees Celsius. Inside these stars, the incredibly high temperatures and pressures result in atoms fusing together and releasing more energy. For much of the 20th century, scientists have investigated whether similar conditions could be created and used on Earth as source of energy.

Over the last 30 years, computing has evolved as a powerful tool in scientific research, including fusion. High performance computers are now routinely being used to advance our understanding of fusion energy, with the goal of harnessing the same power source of the sun in specially built reactors to provide clean and almost unlimited energy. But just as fusion energy is filled with huge potential, high performance computing also presents daunting scientific challenges.

Most of DOE's current research, both in experimental facilities and in computational science, focuses on magnetic fusion research. One approach centers on reactors with doughnut-shaped chambers called tokamaks which would be used to heat ionized gas to about 100 million degrees centigrade, then use powerful magnetic fields to confine and compress the plasma until hydrogen atoms fuse together and release helium and energy. This sustained fusion reaction is known as a "burning plasma." As envisioned, such reactors would generate more energy than they consume. Sustained fusion power generation requires that we understand the detailed physics of the fluid of ions and electrons, or plasma, in a fusion reactor.

With recent advances in supercomputer hardware and numerical algorithm efficiency, large-scale computational modeling can play an important role in the design and analysis of fusion devices. Among the nations engaged in developing magnetic confinement fusion, the U.S. remains the world leader in plasma simulation.

Computational techniques for simulating the growth and saturation of turbulent instabilities in this plasma are critical for developing this understanding of how to control the plasma and hence to develop a successful fusion reactor. Achieving such a goal is a long-term objective and many steps are needed before efficient fusion reactors can be designed and built. A number of smaller experimental reactors have been built in the U.S. and around the world. These facilities are expensive to build and operate, but give scientists valuable information for future designs.

Computational physics research has also helped give fusion scientists important insights into many aspects of plasma confinement, reactor fueling and the effects of turbulence on plasmas. In fact, turbulence has emerged as one of the biggest challenges in magnetic fusion – as the plasmas are heated and confined, turbulence occurs and introduces instabilities, which disrupt the confinement. If the plasmas cannot be confined, the plasmas come into contact with the reactor walls, losing temperature and making fusion impossible.

Under the SciDAC program, computational scientists, applied mathematicians and fusion researchers worked in teams to develop new tools and techniques for advancing fusion research, then using these methods to run more detailed simulations. The result is ever increasing knowledge and understanding about the forces at work within a fusion reactor. This information is being directly applied to the design and construction of ITER, a multinational facility to be built in France.

Since construction costs for ITER have been estimated at $12 billion and once completed, operating costs could be up to $1 million per day, it's critical that the newest, most detailed research findings be applied before the system is completed. Not only will this help minimize the number of costly modifications, but it will also mean a greater likelihood of success.

The results can also be applied on a broader scale to increase our understanding of the many complex physical phenomena in the universe, which we are only starting to understand. Being able to capture and reproduce the phenomenon of fusion on Earth would solve the world's energy problems in an economically and environmentally sustainable manner.

Like other fields, fusion science has developed subfields such as plasma microturbulence theory, magnetohydrodynamics (MHD) and transport theory to study the phenomena which occur, and computational science has greatly advanced research in these areas. Under SciDAC, multi-institution projects were created to advance understanding in specific areas to help advance fusion research around the world.

Center for Extended Magnetohydrodynamic Modeling

The **Center for Extended Magnetohydrodynamic Modeling** project was established to enable a realistic assessment of the mechanisms leading to disruptive and other stability limits in the present and next generation of fusion devices. Rather than starting from scratch, the project built on the work of fusion research teams which developed the NIMROD and M3D codes for magnetohydrodyamic (MHD) modeling. This discipline studies the dynamics of electrically conducting fluids such as plasmas. The goal was to develop these codes to enable a realistic assessment of the mechanisms leading to disruptive and other stability limits in the present and next generation of fusion devices. The main work involves extending and improving the realism of the leading 3D nonlinear magneto-fluid based models of hot, magnetized fusion plasmas, increasing their efficiency, and using this improved capability to pioneer new terascale simulations of unprecedented realism and resolution. As a result, scientists gained new insights into low frequency, long-wavelength nonlinear dynamics

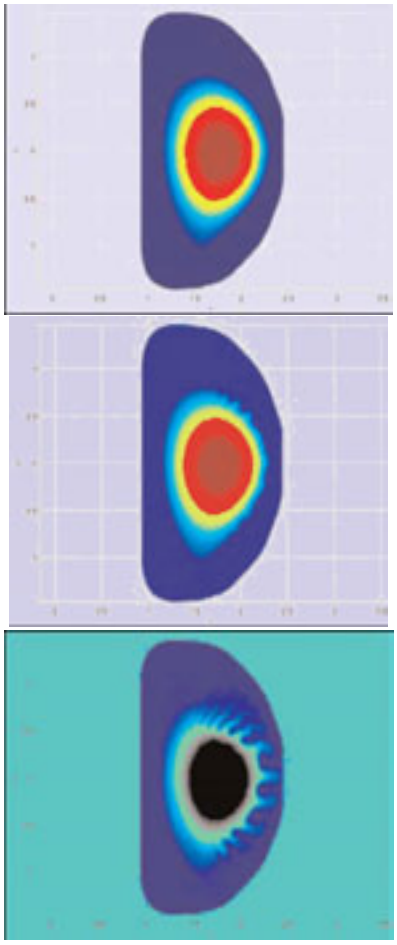


FIGURE 10. Evolution of the temperature during the nonlinear evolution of an edge localized mode in shot 113207.

in hot magnetized plasmas, some of the most critical and complex phenomena in plasma and fusion science. The underlying models are validated through comparisons with experimental results and other fusion codes.

An example of an important fusion problem that is being addressed by the center is the onset and nonlinear evolution of "edge localized modes" (ELMs) and their effect on plasma confinement and the reactor walls. By using the two MHD codes and data from the DIII-D fusion device operated by General Atomics in California, the center was able to achieve a series of scientific milestones in 2005 and 2006. These modes shed thermal energy from the edge of the confinement region and, in their most virulent form, could overheat the walls near the plasma, and may also affect the core plasma. Using the codes advanced under this project, the center team was able to create more extensive simulations of the effects of ELMs than previously possible. The evolution of the temperature during the nonlinear evolution of an ELM in shot 113207 is shown in Figure 10, illustrating the formation of fingerlike structures near the plasma edge with increasingly fine structure as the calculation progresses.

The project also made a number of modifications to the M3D code to improve the accurate representation of a number of conditions in tokamaks.

Principal Investigator: Steve Jardin, Princeton Plasma Physics Laboratory

The Plasma Microturbulence Project

A key goal of magnetic fusion programs worldwide is the construction and operation of a burning plasma experiment. The performance of such an experiment is determined by the rate at which energy is transported out of the hot core (where fusion reactions take place) to the colder edge plasma (which is in contact with material surfaces). The dominant mechanism for this transport of thermal energy is plasma microturbulence.

The development of terascale supercomputers and of efficient simulation algorithms provides a new means of studying plasma microturbulence – direct numerical simulation. Direct numerical simulation complements analytic theory by extending its reach beyond simplified limits. Simulation complements experiment because non-perturbative diagnostics measuring quantities of immediate theoretical interest are easily implemented in simulations, while similar measurements in the laboratory are difficult or prohibitively expensive.

The development of tools in this

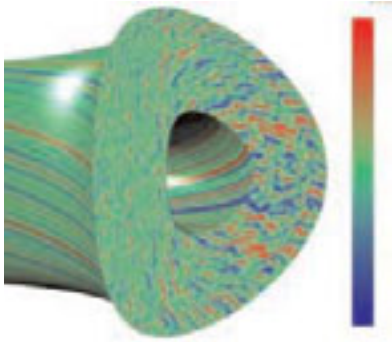


FIGURE 11. The (turbulent) electrostatic potential from a GYRO simulation of plasma microturbulence in the DIII-D tokamak.

project will significantly advance the interpretation of experimental confinement data and will be used to test theoretical ideas about electrostatic and electromagnetic turbulence. By fulfilling the objective of enabling direct comparisons between theory and experiment, direct numerical simulation will lead to improvements in confinement theory and increased confidence in theoretical confinement predictions. **The Plasma Microturbulence Project (PMP)** is addressing this opportunity through a program of code development, code validation, and expansion of the user community.

The project has implemented a number of code improvements for modeling different geometries and multi-species plasma models to simulate both the turbulent electric and magnetic fields in a realistic equilibrium geometry (see Figure 11). The project's global codes are able to simulate plasmas as large as those in present experiments, and the even larger plasmas foreseen in burning plasma experiments.

The project's algorithms scale nearly linearly with processor number to ~1000 processors, which is important as fusion codes are significant users of supercomputing resources at DOE centers. To help the fusion research community benefit from this investment in the GS2 and GYRO codes, the project has engaged researchers in helping to

validate the codes against experimental results. Additionally, project members have conducted training workshops and presented talks on the codes at key fusion research meetings.

Principal Investigator: Bill Nevins, Lawrence Livermore National Laboratory

Center for Gyrokinetic Particle Simulations of Turbulent Transport in Burning Plasmas

The **Center for Gyrokinetic Particle Simulations of Turbulent Transport in Burning Plasmas** consortium was formed in 2004 to develop codes to simulate turbulent transport of particles and energy, and improve the confinement of burning plasmas in fusion reactors. In particular, the project is aimed at developing the capabilities for simulating burning plasma experiments at the scale of ITER, the international thermonuclear experimental reactor which is expected to be the first fusion reactor capable of sustaining a burning plasma when the machine goes on line in about 10 years.

Although fusion scientists have been creating simulation codes to study fusion for more than 30 years, ITER presents two unique challenges, according to Wei-li Lee, head of the center.

First, the size of the reactor and the necessary simulations are large. The ITER will have a major radius of 6.2 meters and a minor radius of two meters, and a correspondingly large confined plasma must be simulated. Second, the temperature inside ITER will be higher than any other fusion reactor. This higher temperature means that new types of physics will be encountered. As a result, new numerical simulation models must be developed.

The new codes must also be created to perform as efficiently as possible so that the larger-scale simulations can be run on the nation's most powerful supercomputers.

The major challenge for the project is to use simulations to better understand and minimize the problem of turbulence in the reactor. At the core of the reactor, the temperatures are at their highest. At the outside edges, the temperatures are lower. As with weather, when there are two regions with different temperatures, the area between is subject to turbulence. This turbulence provides a means for the charged particles in the plasma to move toward the outer edges of the reactor rather than fusing with other particles. If enough particles (and their energy) come into contact with the reactor wall, the particles lose temperature and the fusion reaction cannot be sustained.

Scientists understand that the difference in temperatures as well as densities is what causes the turbulence. But what is still not fully understood is the rate at which particles are transported through the plasma by the turbulence. Experiments show that the particles are transported quite differently than theory suggests. One of the objectives of the center's simulations is to bridge this gap between experiment and theory.

In the simulations, particles will fly around in the plasma according to Newton's laws of motion, although in a much smaller number than will actually be present in the ITER plasma. Algorithms will be developed to follow the path of each simulated particle as it interacts with other particles and is affected by turbulence transport. The results of the simulations will then be compared with experimental results.

To model the particles, the group is using the the gyrokinetic particle-in-cell (PIC) method, first developed in the early 1980s and widely adopted in the 1990s. Gyrokinetic refers to the motion of the particles in a strong magnetic field. In such a field, particles spiral along, with electrons spinning in one direction and ions in the opposite directions. By simplifying the spiraling motion as a charged ring, researchers are able to increase the time steps by several orders of magnitude without sacrificing scientific validity.

The project team also collaborated with Terascale Optimal PDE Simulations Integrated Software Infrastructure Center (TOPS ISICs) established under SciDAC. By integrating other software libraries for solving the equations describing the interaction between the particles, the project team was able to solve a number of physics problems and integrate more realistic physics modules in their simulations. The result is that the simulations are expected to be able to model ITER-scale plasmas by solving a system of equations with millions of unknowns by following billions of particles in the computer.

Principal Investigator: W.W. Lee, Princeton Plasma Physics Laboratory

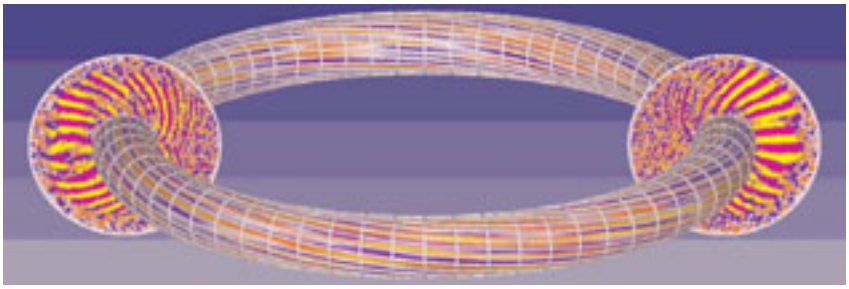


FIGURE 12. Potential contours of microturbulence for a magnetically confined plasma. The finger-like perturbations (streamers) stretch along the weak field side of the poloidal plane as they follow the magnetic field lines around the torus.

Understanding Magnetic Reconnection in Plasmas

The **Center for Magnetic Reconnection Studies (CMRS)** is a multi-university consortium dedicated to physical problems involving magnetic reconnection in fusion, space, and astrophysical plasmas. Understanding magnetic reconnection is one of the principal challenges in plasma physics. Reconnection is a process by which magnetic fields reconfigure themselves, releasing energy that can be converted to particle energies.

The goal of the Magnetic Reconnection project was to produce a unique high performance code to study magnetic reconnection in astrophysical plasmas, in smaller-scale laboratory experiments and in fusion devices. The principal computational product of the CMRS – the Magnetic Reconnection Code (MRC) – is a state-of-the-art, large-scale MHD code for carrying out magnetic reconnection research with accuracy and completeness in 2D and 3D. The MRC is massively parallel and modular, has the flexibility to change algorithms when necessary, and uses adaptive mesh refinement (AMR) (Figure 13). The project team has applied the MRC to a wide spectrum of physical problems: internal disruption (Figure 14) and error-field induced islands in tokamaks, storms in the magnetosphere, solar/stellar flares, and vortex singularity formation in fluids.

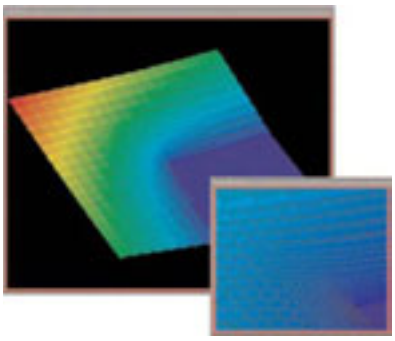


FIGURE 13. AMR allows the MRC code to place refined numerical grids automatically where the fine spatial structures require them, as shown in the figure where sharp spatial gradients at the center are resolved by placing refined grids (see inset for zoom). The MRC code has the capability to refine not only in space but also in time, which is more efficient since one does not need to take unnecessarily small time steps in regions where the fields are smooth.

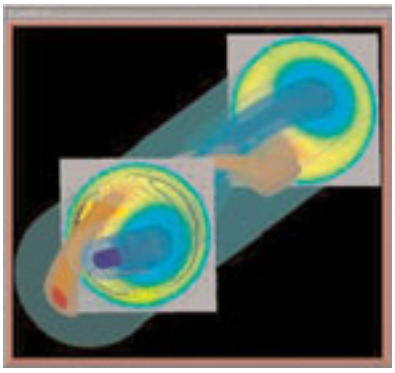


FIGURE 14. A simulation of the so-called kink-tearing instability in tokamaks that can cause internal current disruption and core temperature collapse. The two intertwining helical flux tubes are formed as a result of reconnection, and their 2D projections show magnetic island structure.

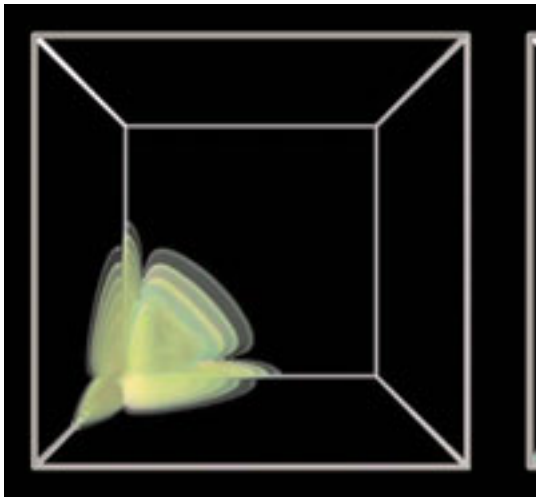
Principal Investigator: Amitava Bhattacharjee, University of New Hampshire

Terascale Computational Atomic Physics for the Edge Region in Controlled Fusion Plasmas

Atomic physics plays a central role in many of the high temperature and high density plasmas found in magnetic and inertial confinement fusion experiments, which are crucial to our national energy and defense interests, as well as in technological plasmas important to the U.S. economic base. In turn, the development of the necessary atomic physics knowledge depends on advances in both experimental and computational approaches. The **Terascale Computational Atomic Physics for the Edge Region in Controlled Fusion Plasmas** project was established to develop a new generation of scientific simulation codes, through a broad ranging collaboration of atomic physicists and computer scientists, which will take full advantage of national terascale computational facilities to address the present and future needs for atomic-scale information for fusion and other plasma environments.

Especially in regard to the needs of fusion, atomic and molecular collisions significantly influence the transport and energy balance in regions crucial for the next step of magnetic confinement fusion development, the divertor and edge of tokamaks. For example, the microscopic modeling of turbulence and transport in magnetic fusion edge plasmas relies heavily on an accurate knowledge of the underlying atomic processes, such as elastic scattering, vibrational energy transfer, mutual neutralization, and dissociative recombination. The transport and atomic conversion of radiation is also at the heart of inertial fusion experiments, where a vast array of electron and photon collision processes, as well as of radiative and electron cascade relaxations, is required to model, diagnose, guide, and understand experiments. In addition, most magnetic fusion diagnostics involve interpretation of observations of the conversion of

FIGURE 15. Accurate modeling of plasmas requires accurate knowledge of atomic processes, such as scattering. This series is from a simulation capturing all scattering processes for the scattering of a wavepack from a helium atom.



fast electron energy to atomic ion light emission, such as in the well known charge exchange recombination spectroscopy. Development of new scientific simulation codes to address these needs will also benefit research involving a huge range of technical, astrophysical, and atmospheric plasmas that also depend on accurate and large scale databases of atomic processes.

Many of the project's atomic collision codes are being implemented on supercomputers at DOE computing centers in California and Tennessee. Results of these code developments will be disseminated openly to the relevant plasma science and atomic physics communities, and will enable new regimes of computation by taking advantage of terascale and successor facilities. All of the atomic collision codes have important applications in a variety of research areas outside controlled fusion plasma science.

Principal Investigator: Michael Pindzola, Auburn University

Numerical Computation of Wave-Plasma Interactions in Multi-Dimensional Systems

In order to achieve the extremely high temperatures – six times hotter than the core of the sun – needed to drive fusion reactions in a tokamak, scientists are studying different approaches to heating. One method involves radio waves, similar to the microwaves used to heat food. As the waves propagate through the plasma, they interact with the ions spinning in the plasma. When the ions' gyro-frequency resonates at the same frequency as the wave, the ions spin up to a very high energy, further heating the plasma.

The goal of **Numerical Computation of Wave-Plasma Interactions in Multi-Dimensional Systems** is to create two-dimensional and three-dimensional simulations of the interactions between the plasma and the waves to make accurate predictions of the processes. The results of these simulations will be used to design and build fusion reactors, including ITER. During the first three years of the project, the main focus was on wave interaction and conversion. What researchers discovered was that under certain conditions, the relatively long waves propagated from an antenna inside the tokamak could be converted to much shorter waves, change characteristics and become much shorter in length. This process is known as "mode conversion." One form of the shorter wave, known as an "ion cyclotron wave," interacts with both the ions and the electrons in the plasma. The project is using two plasma modeling codes – AORSA and TORIC – to study the effects of the

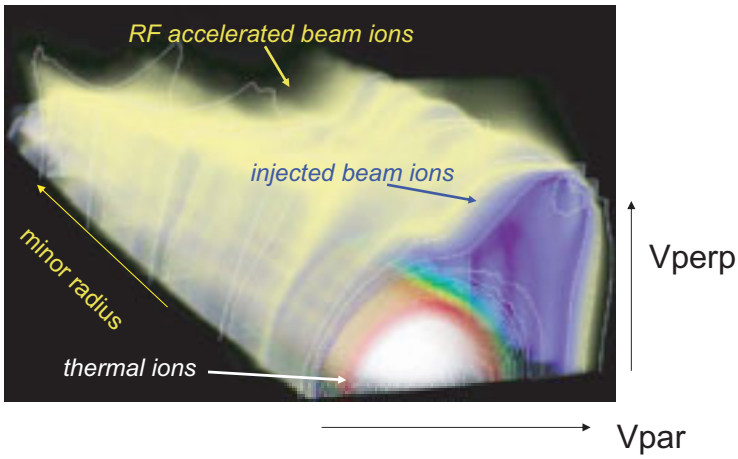
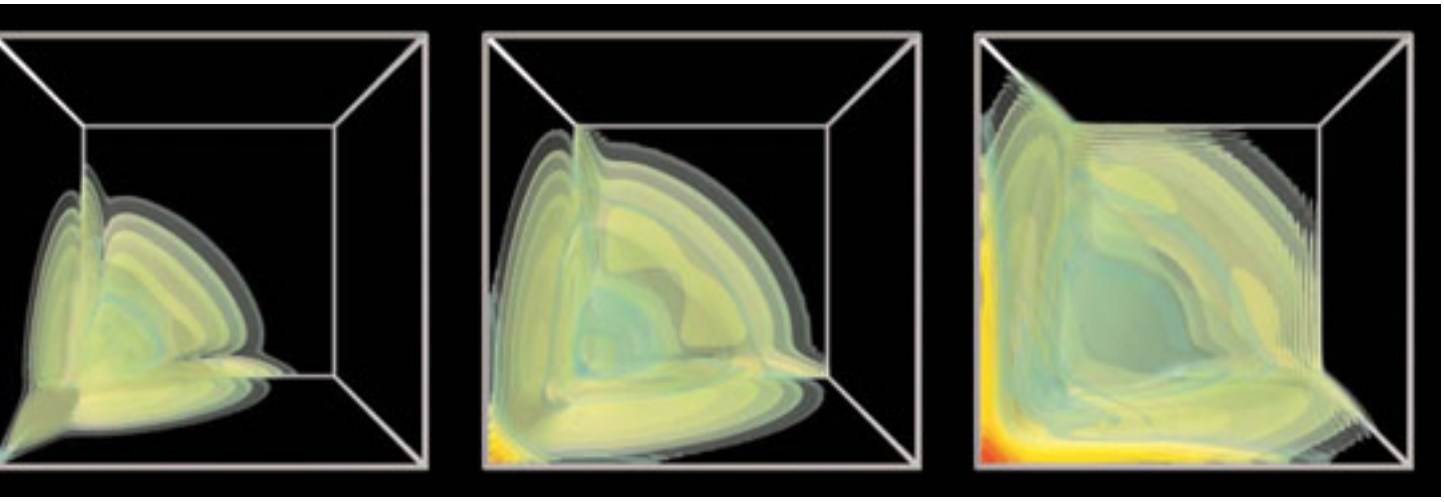


FIGURE 16. Under SciDAC, fusion energy researchers were allocated time on the Cray XT-3 massively parallel supercomputer "Jaguar" at Oak Ridge National Laboratory. By using thousands of processors, the team was able for the first time to run this calculation of how non-thermal ions are distributed in a heated fusion plasma.



ion cyclotron wave. One effect appears to be that the wave drives flows in the plasma which help break up turbulence, thereby improving confinement of the plasma.

In summer 2005, the AORSA global-wave solver was ported to the new Cray XT3 supercomputer at Oak Ridge National Laboratory. The code demonstrated excellent scaling to thousands of processors. Preliminary calculations using 4,096 processors have allowed the first simulations of mode conversion in ITER. Mode conversion from the fast wave to the ion cyclotron wave has been identified in ITER using mixtures of deuterium, tritium and helium-3 at 53 MHz.

A second focus of the project has been on how energies are distributed in the plasma. The simplest type of distribution is known as a Maxwellian distribution, which is used to calculate how energy is distributed in all gases, such as the air in a room. This distribution function was previously the only method in which fusion researchers could calculate wave propagation and absorption. But, when plasmas are heated to very high temperatures, a long tail of particles can form, which represents a non-Maxwellian distribution. Using another code called CQL3D, project team members were able to calculate the new energy distributions. The code was also installed on the Cray XT3 supercomputer along with the AORSA code, and both were programmed to automatically iterate with one another. So, once the new energy distributions were calculated, this data was fed back into the AORSA code to recalculate the heating of the plasma. Once the reheating was simulated, the CQL3D code then calculated the energy distribution. The iterations were repeated until a steady state was reached in the simulation.

The project results, which make key contributions to understanding processes in hot plasmas, were achieved through the scaling of simulation codes and the availability of terascale computing systems.

Principal Investigator: Don Batchelor, Oak Ridge National Laboratory (2001-05), Paul Bonoli, Massachusetts Institute of Technology, (2006-present)

High Energy and Nuclear Physics: Accelerating Discovery from Subatomic Particles to Supernovae

The Office of Science supports a program of research into the fundamental nature of matter and energy through the offices of High Energy Physics and Nuclear Physics. In carrying out this mission, the Office of Science:

- builds and operates large, world-class charged-particle accelerator facilities for the nation and for the international scientific research community;
- builds detectors and instruments designed to answer fundamental questions about the nature of matter and energy; and
- carries out a program of scientific research based on experimental data, theoretical studies, and scientific simulation.

The scale of research ranges from the search for subatomic particles, which are one of the most basic building blocks of matter, to studying supernovae, massive exploding stars which also serve as an astrophysical laboratory in which unique conditions exist that are not achievable on Earth. Under the SciDAC program, projects were launched to advance research in the areas of accelerator science and simulation, quantum chromodynamics and supernovae science.

Advanced Computing for 21st Century Accelerator Science & Technology

Accelerators underpin many of the research efforts of the Office of Science and physics research around the world. From biology to medicine, from materials to metallurgy, from elementary particles to the cosmos, accelerators provide the microscopic information that forms the basis for scientific understanding and applications. Though tremendous progress has been made, our present theory of the physical world is not complete. By tapping the capabilities of the different types of accelerators, including colliders, spallation neutron sources and light sources, scientists are making advances in many areas of fundamental science.

Much of our knowledge of the fundamental nature of matter results from probing it with directed beams of particles such as electrons, protons, neutrons, heavy ions and photons. The resulting ability to "see" the building blocks of matter has had an immense impact on society and our standard of living. Over the last century, particle accelerators have changed the way we look at nature and the universe we live in and have become an integral part of the nation's technical infrastructure. Today, particle accelerators are essential tools of modern science and technology.

For example, about 10,000 cancer patients are treated every day in the United States with electron beams from linear accelerators. Accelerators produce short-lived radioisotopes that are used in over 10 million diagnostic medical procedures and 100 million laboratory tests every year in the United States.

The SciDAC **Accelerator Science and Technology (AST)** modeling project was a national research and development effort aimed at establishing a comprehensive terascale simulation environ-

ment needed to solve the most challenging problems in 21st century accelerator science and technology. The AST project had three focus areas: computational beam dynamics, computational electromagnetics, and modeling advanced accelerator concepts. The newly developed tools are now being used by accelerator physicists and engineers across the country to solve the most challenging problems in accelerator design, analysis, and optimization.

An accelerator generates and collects billions of elementary particles, such as electrons, positrons or protons, into a limited space, then accelerates these particles in a beam toward a target – another beam of particles or devices for producing radiation or other particles. In the process of acceleration, the energy of every particle in the beam is increased tremendously. In order to advance elementary particle physics into regions beyond our present knowledge, accelerators with larger final beam energies approaching the tera electron volt (TeV) scale are required.

The Department of Energy operates some of the world's most powerful accelerators, including a three-kilometer-long linear accelerator at the Stanford Linear Accelerator Center (SLAC) in California, the Tandem Linac Accelerator System at Argonne National Laboratory (ANL) in Illinois, the Tevatron at Fermilab in Illinois, the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory (BNL) in New York, the Continuous Electron Beam Accelerator Facility in Virginia and the Holifield Radioactive Ion Beam Facility at Oak Ridge National Laboratory (ORNL) in Tennessee. DOE-operated light sources are the Advanced Light Source at Lawrence Berkeley National Laboratory in California, the Advanced Photon Source at ANL, the National Synchrotron Light Source at BNL and the Stanford Synchrotron Radiation Laboratory at SLAC. Neutron sources include the Spallation Neutron Source at ORNL and the Los Alamos Neutron Science Center at Los Alamos National Laboratory in New Mexico. While accelerators can be of different configurations with different capabilities, most use radio frequencies (RF) to accelerate the particles. In order to experimentally pursue the quest for the grand unified theory ever more powerful accelerators are needed. Such massive facilities are costly to build and require specialized infrastructure.

The long-term future of experimental high-energy physics research using accelerators depends on the successful development of new acceleration methods which can accelerate particles to even higher energy levels per acceleration length (known as the accelerating gradient). In the past, this was achieved by building a longer accelerator, an approach which faces practical limits in space and cost.

Since building such accelerators is time-consuming and expensive, scientists are using computer simulations to increasing our understanding of the physics involved and to help improve the design for more efficient acceleration. High-resolution, system-scale simulation utilizing terascale computers such as the IBM SP supercomputer at NERSC, has been made possible by SciDAC-supported code development efforts and collaborations with the SciDAC ISICs. This team-oriented approach to computing is beginning to make a qualitative difference in the R&D of major DOE accelerators, existing or planned.

Beam Dynamics: Maximizing Scientific Productivity

The AST project has had a major impact on computational beam dynamics and the design of particle accelerators. Thanks to SciDAC, accelerator design calculations that were once thought impossible are now carried out routinely. SciDAC accelerator modeling codes are being used to get the most science out of existing facilities, to produce optimal designs for future facilities, and to explore advanced accelerator concepts that may hold the key to qualitatively new ways of accelerating charged particle beams. Here are some high-

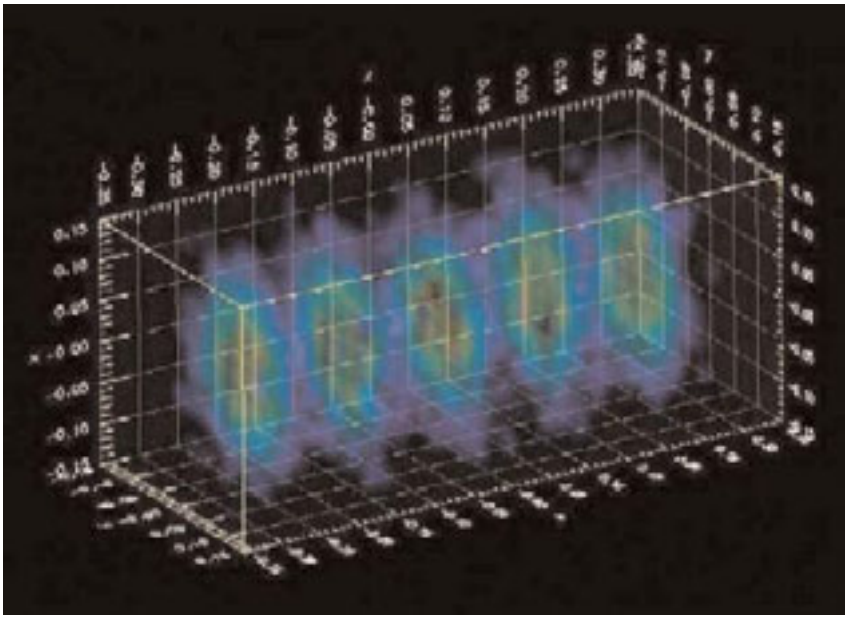


FIGURE 17. This simulation of the Fermi Booster, a synchrotron accelerator ring, was created using the Synergia software developed under SciDAC.

lights from the AST project Beam Dynamics focus area in regard to algorithm development, software development, and applications.

Particle simulation methods have been among the most successful and widely used methods in computational beam physics, plasma physics and astrophysics. Under the AST project a comprehensive, state-of-the-art set of parallel particle-in-cell (PIC) capabilities has been developed, including:

- IMPACT: An integrated suite of codes originally developed to model high intensity ion linacs, IMPACT's functionality has been greatly enhanced so that it is now able to model high brightness electron beam dynamics, ion beam dynamics and multi-species transport through a wide variety of systems.
- BeamBeam3D: A code for modeling beam-beam effects in colliders. This code contains multiple models and multiple collision geometries and has been used to model the Tevatron, Positron-Electron Project (PEP)-II, Relativistic Heavy Ion Collider (RHIC), and Large Hadron Collider (LHC) accelerators.
- MaryLie/IMPACT: A code that combines the high-order optics modeling capabilities of the MaryLie Lie algebraic beam transport code with the parallel PIC capabilities of IMPACT. It is used to model space-charge effects in large circular machines such as the ILC damping rings.
- Synergia: A parallel beam dynamics simulation framework, Synergia combines multiple functionality, such as the space-charge capabilities of IMPACT and the high-order optics capabilities of MXYZPLT, along with a "humane" user interface and standard problem description.

Crucial to the development of the AST project's codes has been the collaboration with the SciDAC ISICs and with other DOE-supported activities. In some cases, the use of advanced algorithms has led to applications running up to 100 times faster.

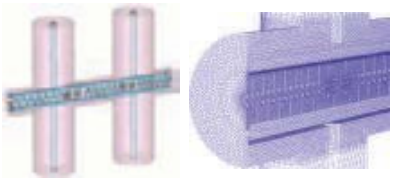


FIGURE 18. (Left) A model of RIA's hybrid RFQ and (Right) an enlarged portion of the corresponding Omega3P mesh.

SciDAC AST beam dynamics codes have been applied to several important projects within the DOE Office of Science. Examples include:

- existing colliders, including the Tevatron, RHIC and PEP-II
- future colliders such as the LHC currently under construction
- proposed linear colliders such as the International Linear Collider (ILC)
- high intensity machines, including the Fermilab booster and the Spallation Neutron Source (SNS) ring under construction
- linacs for radioactive ion beams, such as the proposed Rare Isotope Accelerator (RIA)
- electron linacs for fourth-generation light sources, such as the Linac Coherent Light Source now under construction.

Electromagnetic Systems Simulation: Prototyping through Computation

The AST project has supported a well-integrated, multi-institutional, multi-disciplinary team to focus on the large-scale simulations necessary for the design and optimization of electromagnetic systems essential to accelerator facilities. As a result, an increasing number of challenging design and analysis problems are being solved through large-scale simulations, benefiting such projects as the PEP-II, Next Linear Collider (NLC), and the proposed ILC and RIA.

Central to these efforts is a suite of 3D parallel electromagnetic design codes: Omega3P, Tau3P, Track3P, S3P and T3P. Collaborations with SciDAC ISICs led to a number of improvements in the codes which have not only increased the speed and accuracy of the codes up to tenfold, but have expanded their capabilities for solving more complicated problems of importance to present and future accelerators. The codes have been used to advance a number of DOE accelerator projects, including the ILC, PEP-II, NLC, RIA and LCSS.

For example, the AST electromagnetic codes were applied to the PEP-II facility, which now operates with twice the luminosity of the original design and is aiming for another twofold increase. However, beam heating in the interaction region (IR) could limit the accelerator from meeting that goal. The Tau3P code has been used to calculate the heat load in the present design. Higher currents and shorter bunches of particles will require modifications to the IR to reduce the increased heating. T3P will be able to model the entire IR geometry and to simulate the actual curved beam paths in any new IR design.

The proposed RIA, which is ranked third in the Office of Science's 20-year Science Facility Plan, requires design of a variety of radio frequency quadropole (RFQ) cavities (Figure 18) for its low-frequency linacs. Due to lack of accurate predictions, tuners are designed to cover frequency deviations of about 1 percent. With Omega3P, frequency accuracy of 0.1 percent can be reached, significantly reducing the number of tuners and their tuning range. Parallel computing will play an important role in prototyping RIA's linacs and help reduce their costs.

Modeling Advanced Accelerators: Miniaturizing Accelerators from Kilometers to Meters

The long-term future of experimental high-energy physics research using accelerators is partly dependent on the successful development of novel ultra high-gradient acceleration methods. New acceleration techniques using lasers and plasmas have already been shown to exhibit gradients (or acceleration) and focusing forces more than 1000 times greater than conventional technology. The challenge is to control these high-gradient systems and then to string them together. Such technologies would not only enable a cost-effective path to the outermost reaches of the high-energy frontier, but could also lead to the development of ultra-compact accelerators. Such compact accelerators could benefit science, industry and medicine by shrinking large facilities to a much reduced size and allowing them to be built nearer research organizations, high-tech businesses and medical centers.

Under the AST Project, the Advanced Accelerator effort has emphasized developing a suite of fully parallel 3D electromagnetic PIC codes. The codes have been benchmarked against each other and their underlying algorithms, as well as against experiments. The resulting codes provide more realistic models, which are being applied to advanced accelerators as well as more mainstream problems in accelerator physics. Furthermore, the effort has included running these codes to plan and interpret experiments and to study the key physics that must be understood before a 100+ GeV collider based on plasma techniques can be designed and tested.

In some advanced accelerator concepts a drive beam, either an intense particle beam or laser pulse, is sent through a uniform plasma. The space charge or radiation pressure creates a space-charge wake on which a trailing beam of particles can surf. To model such devices accurately usually requires following the trajectories of individual plasma particles. Therefore, the software tools developed fully or partially under this project – OSIRIS, VORPAL, OOPIC, QuickPIC and UPIC – rely on the PIC techniques.

Among the major accomplishments are:

The development of UPIC: Using highly optimized legacy code, a modern framework for writing all types of parallelized PIC codes including electrostatic, gyrokinetic, electromagnetic, and quasi-static has been developed. The UPIC Framework has obtained 30 percent of peak speed on a single processor and 80 percent efficiency on well over 1,000 processors. It is used across both the accelerator and fusion SciDAC projects.

The rapid construction of QuickPIC: The development of QuickPIC is a success story for the rapid construction of a new code using reusable parallel code via a SciDAC team approach. The basic equations and algorithms were developed from a deep understanding of the underlying physics involved in plasma and/or laser wakefield acceleration while the code was constructed rapidly using the UPIC Framework. In some cases, QuickPIC can completely reproduce the results from previous algorithms with a factor of 50 to 500 savings in computer resources. It is being used to study beam-based science in regimes not accessible before.

Rapidly adding realism into the computer models: The large electromagnetic fields from the intense drive beams can field ionize a gas, forming a plasma. Early SciDAC research using two-dimensional codes revealed that this self-consistent formation of the plasma from the drive beam needs to be included in many cases. Via the SciDAC team approach, ionization models have been added and benchmarked against each other in the fully three-dimensional PIC codes, VORPAL and OSIRIS.

Extending the plasma codes to model the electron-cloud instability: The electron cloud instability is one of the major obstacles for obtaining the design luminosity in circular accelerators, storage rings and damping rings. A set of modules has been written for QuickPIC that models circular orbits under the influence of external focusing elements. This new software tool has already modeled 100,000 km of beam

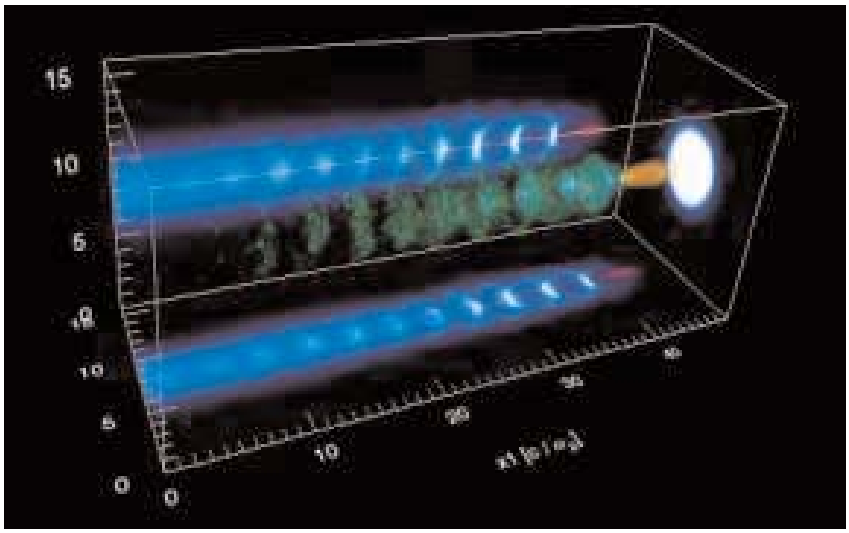


FIGURE 19. 3D afterburner simulation results.

propagation of the SPS machine at CERN. It is a major improvement over previously existing tools for modeling electron cloud interactions.

Applying the suite of codes to discover new accelerator science: The suite of PIC codes has been used to model particle beam accelerator experiments at the Stanford Linear Accelerator Center and the laser-plasma experiments at the L'OASIS lab at Lawrence Berkeley National Laboratory. They have also been used to study key physics issues related to the afterburner concept, in which the energy of an existing beam from an accelerator is doubled with gradients near 10 GeV/m. An example is shown in Figure 19 where the beam and plasma density is shown from a three-dimensional simulation for the afterburner, including field ionization.

Principal Investigators: Robert Ryne, Lawrence Berkeley National Laboratory, and Kwok Ko, Stanford Linear Accelerator Center

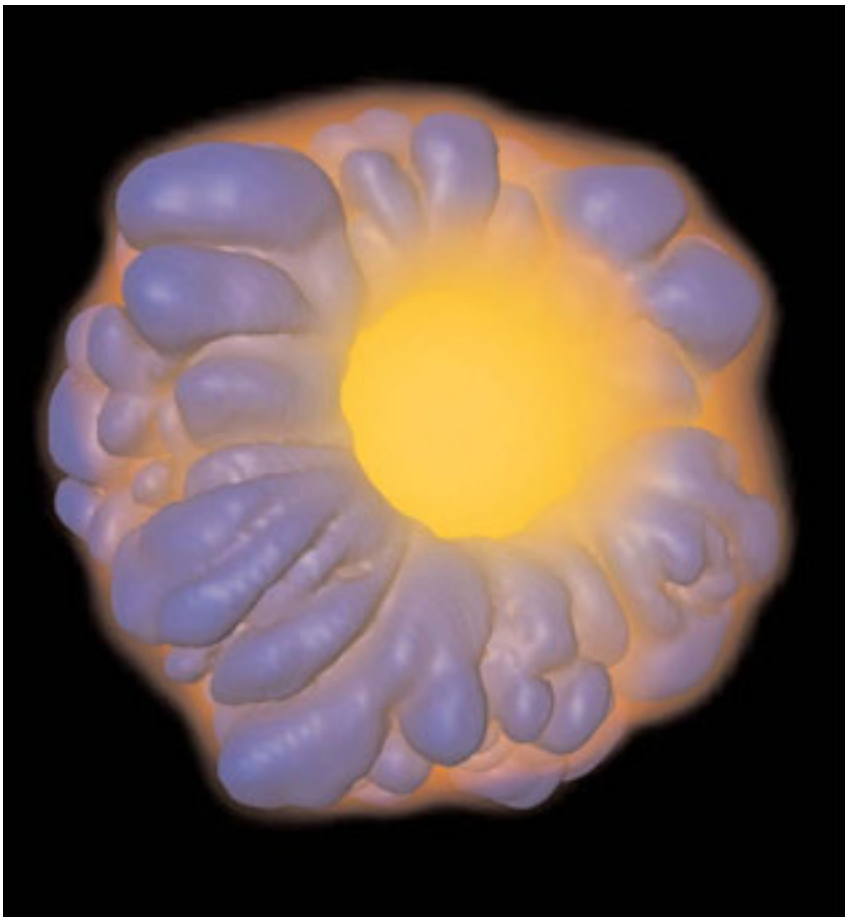


FIGURE 20. A full star 3D model of a Type Ia supernova explosion

Supernovae Science: Getting the Inside Story on How Stars Explode

While supernovae are awesome in their own right – these exploding stars expire in flashes brighter than whole galaxies – they can also provide critical information about our universe. Because of their regular brightness, Type Ia supernovae are used as astronomical "standard candles" for cosmic distances and the expansion of the universe. Supernovae are also helping scientists gain a better understanding of the dark energy thought to make up 75 percent of the universe. And finally, supernovae are also the source of the heavy elements in our universe, as well as prolific producers of neutrinos, the most elusive particles so far discovered.

The best perspective from which to observe supernovae is from a telescope mounted on a satellite. But earth-bound supercomputers are also proving to be powerful tools for studying the forces behind the most powerful explosions in the universe. To help understand the conditions which lead to supernovae explosions, the SciDAC program launched two projects – the Supernova Science Center and the Terascale Supernova Initiative.

The Supernova Science Center

The **Supernova Science Center (SNSC)** was established with the objective of using numerical simulations to gain a full understanding of how supernovae of all types explode and how the elements have been created in nature. These computational results are then compared with astronomical observations, including the abundance patterns of elements seen in our own sun.

The explosions both of massive stars as "core-collapse" supernovae and of white dwarfs as "thermonuclear" supernovae (also called Type Ia) pose problems in computational astrophysics that have challenged the community for decades. Core-collapse supernovae require at least a two- (and ultimately three-) dimensional treatment of multi-energy-group neutrinos coupled to multi-dimensional hydrodynamics. Type Ia explosions are simulation problems in turbulent (nuclear) combustion.

During its first five years, the SNSC focused on forging the interdisciplinary collaborations necessary to address cutting-edge problems in a field that couples astrophysics, particle physics, nuclear physics, turbulence theory, combustion theory

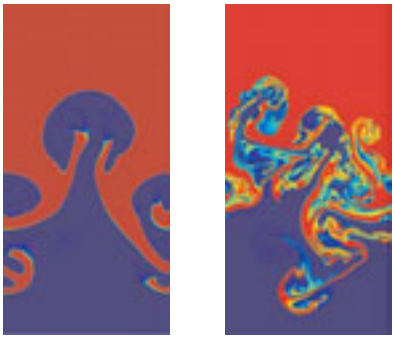


FIGURE 21. A burning Rayleigh-Taylor unstable flame front calculated for conditions inside a Type Ia supernova using the LBNL low-Mach-number, adaptive-mesh code.

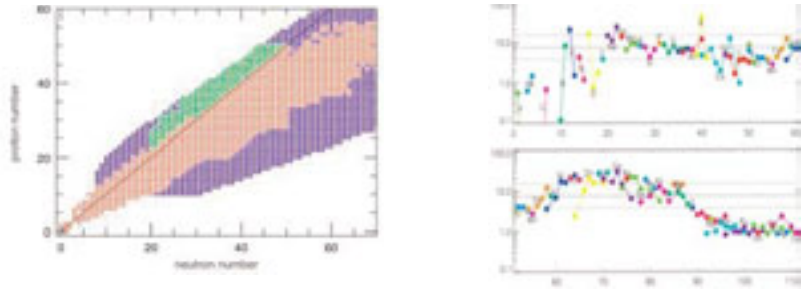


FIGURE 22. A portion (Z < 60) of the isotopes included in SNSC's nuclear reaction library – one of the most extensive in the world. Right: nucleosynthesis averaged over mass for a set of massive supernovae from 12 to 100 times the mass of the sun.

and radiation transport. The project team also worked to develop and modify the necessary computer codes to incorporate the physics efficiently and do exploratory calculations.

Examples of these alliances are the chemical combustion groups at Lawrence Berkeley and Sandia National Laboratories; the NSF's Joint Institute for Nuclear Astrophysics (JINA); and radiation transport and nuclear physics experts at Los Alamos and Lawrence Livermore National Laboratories. With LBNL, the team applied codes previously optimized to study chemical combustion on large parallel computers to novel problems in nuclear combustion in white dwarf stars (Figure 21), carrying out for the first time fully resolved studies of the flame in both the "flamlet" and "distributed" regimes.

The project team worked with JINA to develop a standardized library of nuclear data for application to the study of nucleosynthesis in stars, supernovae and X-ray bursts on neutron stars (Figure 22).

The SNSC is also tapping the expertise of the SciDAC ISICSs. For example, the TOPS ISIC is working with members of the team to produce more efficient solvers, with a goal of increasing the performance of the multi-dimensional codes by a factor of 10.

Other SNSC achievements include:

- Carrying out the first 3D, full-star simulation of core collapse and explosion. The project also carried out simulations in 2D with multi-group neutrino transport of the collapse, bounce, and early post-bounce evolution. Recently a new supernova mechanism was discovered, powered by neutron star vibrations.
- Developing and using 3D adaptive mesh relativistic hydrocodes to model the production of gamma-ray bursts in massive stars, which led to the prediction of a new kind of high energy transient – cosmological x-ray flashes, which were later discovered. (An image from this model appears on the cover of this report.)
- Carrying out the world's best simulations of Type I X-ray bursts on neutron stars. The nuclear physics of these explosions is a primary science goal of DOE's proposed Rare Isotope Accelerator.
- Calculating the ignition of the nuclear runaway in a white dwarf star becoming a Type Ia supernova, which showed that the ignition occurs off-center. Other research has shown that the resulting supernova depends critically upon whether it is ignited centrally or at a point off center. This issue of how the white dwarf ignites has become the most debated and interesting issue in Type Ia supernova modeling today.

The Terascale Supernova Initiative: Shedding New Light on Exploding Stars

Established to "shed new light on exploding stars," SciDAC's **Terascale Supernova Initiative (TSI)** is a multidisciplinary collaboration which will use modeling of integrated complex systems to search for the explosion mechanism of core-collapse supernovae – one of the most important and challenging problems in nuclear astrophysics. The project team, which includes scientists, computer scientists and mathematicians, will develop models for core collapse supernovae and enabling technologies in radiation transport, radiation hydrodynamics, nuclear structure, linear systems and eigenvalue solution and collaborative visualization. These calculations, when carried out on terascale machines, will provide important theoretical insights and support for the large experimental efforts in high energy and nuclear physics.

A key focus of the TSI project is understanding what causes the core of a large star to collapse. When the star runs out of fuel, pressures in the core build and fuse elements together, leading to accelerating combustion. At the end, only iron is left at

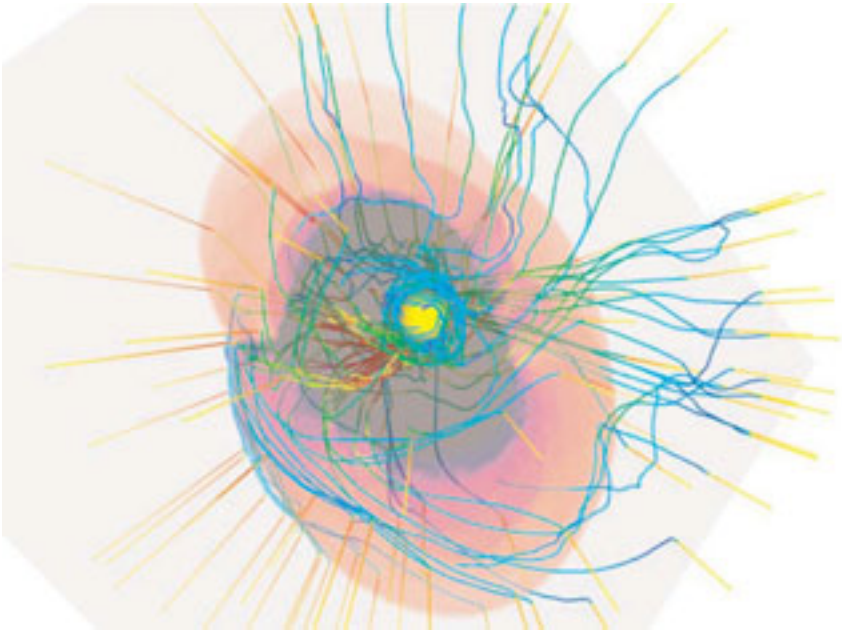


FIGURE 23. This image illustrates the stable rotational flow found in recent 3D simulations of the SASI, computed on the Cray X1 at NCCS. The streamlines show the inward flow of the core being deflected by the nascent supernova shock and ultimately wrapping around the inner core.

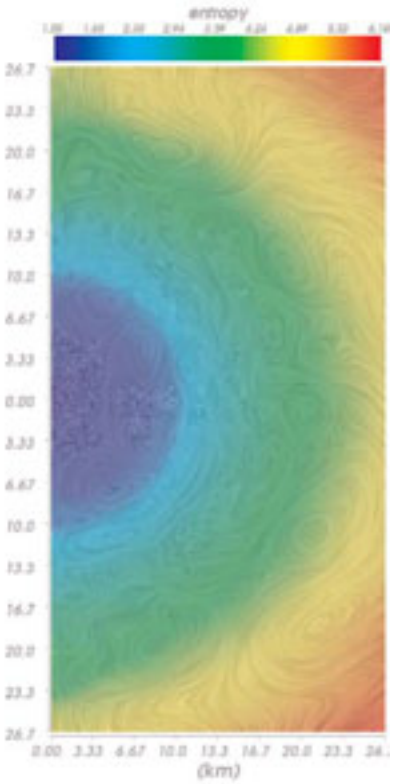


FIGURE 24. A closeup look at a proto-neutron star model, shown at about 32 ms following core bounce, as calculated by the 2D radiation-hydrodynamic code, V2D. The distance scale is given in kilometers. This view focuses on the inner 25 km of a model that extends nearly 6000 km into the oxygen shell. The figure is color mapped by entropy. Velocity direction is shown using an LEA texture map. Convective motion can be seen to encompass the entire inner core. However, even at this early stage of evolution, vigorous motion has ceased, leaving this region moving at only a few percent of the sound speed.

the core and fusion stops. As the iron core grows, gravitational forces eventually cause the core to implode, or collapse, leading to an explosion. This explosion creates both heavy elements and neutrinos. Once the core can no longer collapse any more, it "bounces" back and sends a shock wave through the external layers of the star. If the shock wave kept going, it would lead to the supernova blast. But, for reasons still not understood, the shock wave stalls before it can trigger the explosion in current simulations. TSI researchers are formulating new ways to examine critical events in the supernova core within the first second after the core bounces. One theory is that neutrino heating helps re-energize the stalled shock.

The TSI project created a series of 3D hydrodynamic simulations showing the flow in a stellar explosion developing into a strong, stable, rotational flow (streamlines wrapped around the inner core). The flow deposits enough angular momentum on the inner core to produce a core spinning within a period of only a few milliseconds. This new ingredient of core-collapse supernovae, which can only be modeled in full 3D simulations, may have a dramatic impact on both the supernova mechanism itself and on the neutron star left behind by the supernova event. The strong rotational flow below the supernova shock leads to an asymmetric density distribution that can dramatically alter the propagation of neutrinos, which may in turn enhance the efficiency of a neutrino-driven shock. This rotational flow will also provide a significant source of energy for amplifying any pre-existing magnetic fields through the magneto-rotational instability. Finally, the accretion of the rotational flow onto the central core can spin up the proto-neutron star to periods of order tens of milliseconds, consistent with the inferred rotational period of radio pulsars at birth.

Other team members were able to carry out the most physically detailed 2D core-collapse supernova simulations to date using preconditioners, which are approximating techniques for speeding up linear solvers. Earlier simulations used a gray approximation, which assumes a shape of the energy distribution spectrum for neutrinos. In contrast, the TSI simulations using the V2D code computed the energy spectra of the neutrinos, which change with time and with position as the supernova evolves. That's far more realistic, but requires extensive computing power. With SciDAC providing access to terascale supercomputers, the team was able to solve the problem.

Using V2D, initial studies have shown a number of new results and

confirmed some results reported by others. These include a much earlier onset of post-bounce radiative-hydrodynamic instabilities and development of a hydrodynamically unstable region that quickly grows to engulf the entire region inside the core-bounce shock wave, including both neutrino-transparent regions as well as the proto-neutron star where material is opaque to neutrinos. The most detailed simulations have proceeded to about 35 milliseconds following core bounce, and the team is working to extend these simulations to significant fractions of a second and beyond.

Interaction between astrophysicists and nuclear physicists on the TSI team resulted in the first stellar core collapse simulations to implement a sophisticated model for the stellar core nuclei. The increased sophistication in the nuclear models led to significant quantitative changes in the supernova models, demonstrating that both the microphysics and the macrophysics of core collapse supernovae must be computed with care. The significance of this work led to the publication of two associated Physical Review Letters, one focusing on the astrophysics and one focusing on the nuclear physics. The work has also motivated nuclear experiments to measure nuclear cross-sections as a way to validate the nuclear models used in supernova simulations.

In the last few years experiments and observations have revealed that neutrinos have mass and can change their flavors (electron, muon and tau). This development could turn out to be significant for the core collapse supernova explosion problem, for associated nucleosynthesis and for a neutrino signal detection. Although some experimental results indicate that neutrinos would not be able to transform to the point where they could affect the shock wave, the TSI team has mapped out scenarios in which the behavior of neutrinos could in principle affect the dynamics and nucleosynsthesis deep inside the supernova environment.

National Computational Infrastructure for Lattice Gauge Theory: Accomplishments and Opportunities

The long-term goals of high energy and nuclear physicists are to identify the fundamental building blocks of matter, and to determine the interactions among them that lead to the physical world we observe. The fundamental theory of the strong interactions between elementary particles is known as quantum chromodynamics, or QCD. The strong force is one of four fundamental forces in nature, and provides the force to bind quarks to construct protons and neutrons, which account for about 98 percent of the matter in nature.

The objective of the SciDAC **National Computational Infrastructure for Lattice Gauge Theory** project is to construct the computational infrastructure needed to study QCD. Nearly all high energy and nuclear physicists in the United States working on the numerical study of QCD are involved in this project, and the infrastructure created will be available to all. The project includes the development of community software for the effective use of terascale computers, and research and development of specialized computers for the study of QCD.

The Department of Energy supports major experimental, theoretical and computational programs aimed at reaching these goals. Remarkable progress has been made through the development of the Standard Model of high energy and nuclear physics, which provides fundamental theories of the strong, electromagnetic and weak interactions. This progress has been recognized through the award of Nobel Prizes in Physics for the development of each of the components of the Standard Model: the unified theory of weak and electromagnetic interactions in 1979, and QCD, the theory of the strong interactions, in 1999 and 2004. However, our understanding of the Standard Model is incomplete because it has proven extremely difficult to determine many of the most interesting predictions of QCD, those that involve the strong coupling regime of the theory. To do so requires large scale numerical simulations within the framework of lattice gauge theory.

The scientific objectives of lattice QCD simulations are to understand the physical phenomena encompassed by QCD, and to make precise calculations of the theory's predictions. Lattice QCD simulations are necessary to solve fundamental problems in high energy and nuclear physics that are at the heart of DOE's large experimental efforts in these fields. Major goals of the experimental programs in high energy and nuclear physics on which lattice QCD simulations can have an important impact are to: (1) verify the Standard Model or discover its limits; (2) understand the internal structure of nucleons and other strongly interacting particles and (3) determine the properties of strongly interacting matter under extreme conditions, such as those that existed immediately after the Big Bang and are produced today in relativistic heavy–ion experiments. Lattice QCD calculations are essential to research in all of these areas.

The numerical study of QCD requires very large computational resources, and has been recognized as one of the grand challenges of computational science. The advent of terascale computing, coupled with recent improvements in the formulation of QCD on the lattice, provide an unprecedented opportunity to make major advances in QCD calculations. The infrastructure created under this SciDAC grant will play a critical role in enabling the U.S. lattice QCD community to take advan-

tage of these opportunities. In particular, the hardware research and development work provides the groundwork for the construction of dedicated computers for the study of QCD, and the community software will enable highly efficient use of these computers and the custom designed 12,228-node QCDOC computer recently constructed at Brookhaven National Laboratory (BNL).

Software Development

The project's software effort has created a unified programming environment, the QCD Application Programming Interface (QCD API), that enables members of the U.S. lattice gauge theory community to achieve high efficiency on terascale computers, including the QCDOC, commodity clusters optimized for QCD, and commercial supercomputers. Design goals included enabling users to quickly adapt codes to new architectures, easily develop new applications and preserve their large investment in existing codes.

The QCD API is an example of an application-specific code base serving a national research community. It exploits the special features of QCD calculations that make them particularly well suited to massively parallel computers. All the fundamental components have been implemented and are in use on the QCDOC hardware at BNL, and on both the switched and mesh architecture Pentium 4 clusters at Fermi National Accelerator Labor-atory (FNAL) and Thomas Jefferson National Accelerator Facility (JLab). The software code and documentation are publicly available via the Internet.

Hardware Research and Development

The second major activity under the Lattice QCD SciDAC grant has been the design, construction and operation of commodity clusters optimized for the study of QCD. This work has taken place at FNAL and JLab. The objective has been to provide computing platforms to test the QCD API, and to determine optimal configurations for the terascale clusters planned for FY 2006 and beyond.

The clusters that have been built are being used to carry out important research in QCD. The bottleneck in QCD calculations on clusters, as on commercial supercomputers, is data movement, not CPU performance. QCD calculations take place on four-dimensional space-time grids, or lattices. To update variables on a lattice site, one only needs data from that site and a few neighboring ones. The standard strategy is to assign identical sub-lattices to each processor. Then, one can update lattice points on the interior of the sub-lattices, for which all the relevant neighbors are on the same processor, while data is being collected from a few neighboring processors to update lattice sites on the sub-lattice boundaries. This strategy leads to perfect load balancing among the processors, and, if the computer and code are properly tuned, to overlap of computation and communications.

FIGURE 25. Under SciDAC's Lattice QCD project, two computer clusters were developed for use by the lattice gauge theory community. The system on the left is the 6n cluster at DOE's Jefferson Lab. At the right is the QCDOC computer, constructed at Brookhaven National Laboratory by a group centered at Columbia University. The RBRC computer on the right side of the photo was funded by the Riken Research Institute in Japan. Together, the two systems have a peak speed of 20 teraflop/s.

Building a Better Software Infrastructure for Scientific Computing

Infrastructure usually brings to mind images of physical structures such as roads, bridges, power grids and utilities. But computers also rely on an infrastructure of processors, software, interconnects, memory and storage, all working together to process data and accomplish specific goals. While personal computers arrive ready to use with easy-to-install software, scientists who rely on supercomputers have typically developed their own software, often building on codes that were developed 10 or 20 years ago.

As supercomputers become more powerful and faster, computational scientists are seeking to adapt their codes to utilize this computing power to develop ever more detailed simulations of complex problems. Other scientists are using supercomputing centers to store, analyze and share data from large experimental facilities, such as particle colliders or telescopes searching deep space for supernovae.

But scaling up applications to run on the newest terascale supercomputers, which can perform tens of trillions of calculations per second, presents numerous challenges. First, many of these scientific applications were written by researchers over the course of years or decades for older computers with tens or hundreds of processors and may not be easily adapted to run on thousands or tens of thousands of processors. Second, in some cases, scaling an existing application to run on more processors can actually slow down the run time as the communication between processors bogs down. Because these "legacy codes" often represent significant intellectual investment aimed at solving very specific problems, scientists are reluctant to start anew in developing new codes. Finally, even when applications can be adapted to run more efficiently on one computer architecture, they may not achieve similar performance on another type of supercomputer, an issue of growing importance as supercomputing centers increasingly share their computers to meet the growing demand for greater computing capability. Understanding computer performance and developing tools to enhance this performance enables scientists to scale up their codes to study problems in greater detail for better understanding.

To help bridge the gap between these legacy codes and terascale computing systems, SciDAC established seven Integrated Software Infrastructure Centers, or ISICs, which brought together experts from government computing centers, scientific disciplines and industry to approach the problems from different perspectives to create broadly applicable solutions. In many cases, computing tools originally developed and refined for one type or problem were found to be useful in solving problems in other scientific areas, too. As a result of these focused efforts, scientists can now draw on a wide range of tools and techniques to ensure their codes perform efficiently on supercomputers of varying sizes, with different architectures and at various computing centers.

An important emphasis of SciDAC is that the ISIC teams worked with other projects to enable the effective use of terascale systems by SciDAC applications.

Specifically, the ISICS addressed the need for:

- new algorithms which scale to parallel systems having thousands of processors
- methodology for achieving portability and interoperability of complex high performance scientific software packages
- operating systems tools and support for the effective management of terascale and beyond systems, and
- effective tools for feature identification, data management and visualization of petabyte-scale scientific datasets.

The result is a comprehensive, integrated, scalable, and robust high performance software infrastructure for developing scientific applications, improving the performance of existing applications on different supercomputers and giving scientists new techniques for sharing and analyzing data.

Applied Mathematics ISICs

Three applied mathematics ISICs were created to develop algorithms, methods and mathematical

libraries that are fully scalable to many thousands of processors with full performance portability.

An Algorithmic and Software Framework for Applied PDEs (APDEC)

Many important DOE applications can be described mathematically as solutions to partial differential equations (PDEs) at multiple scales. For example, combustion for energy production and transportation is dominated by the interaction of fluid dynamics and chemistry in localized flame fronts. Fueling of magnetic fusion devices involves the dispersion of material from small injected fuel pellets. The successful design of high-intensity particle accelerators relies on the ability to accurately predict the space-charge fields of localized beams in order to control the beams, preserve the beam emittance and minimize particle loss.

The goal of the **Algorithmic and Software Framework for Applied PDEs (APDEC) ISIC** project has been to develop a high performance algorithmic and software framework for multiscale problems based on the use of block-structured adaptive mesh refinement (AMR) for representing multiple scales. In this approach, the physical variables are discretized on a spatial grid consisting of nested rectangles of varying resolution, organized into blocks. This hierarchical discretization of space can adapt to changes in the solution to maintain a uniform level of accuracy throughout the simulation, leading to a reduction in the time-to-solution by orders of magnitude compared to traditional fixed-grid calculations with the same accuracy. In short, AMR serves as a computational microscope, allowing scientists to focus their computing resources on the most interesting aspects of a problem. The resulting algorithms have enabled important scientific discoveries in a number of disciplines.

The APDEC center has been involved with the development of applications in the areas of combustion simulations, magnetohydrodynamic (MHD) modeling for fusion energy reactors called tokamaks, and modeling particle accelerators. In combustion, the center developed new, more efficient simulation methods for solving chemically reacting fluid flow problems. These algorithms and software have been used to study a variety of problems in the combustion of hydrocarbon fuels, as well as providing the starting point for the development of a new capability for simulating nuclear burning in Type 1a supernovae.

In the area of fusion research, the center developed AMR codes to investigate a variety of scientific problems, including tokamak fueling (Figure 1) and magnetic reconnection, which can help in the design of fusion reactors for future energy production.

In the area of accelerator modeling, two new capabilities were developed: an AMR-particle-in-cell (AMR-PIC) algorithm that has been incorporated into the MLI and Impact beam dynamics codes (Figure 2); and a prototype capability for use in simulating gas dynamics

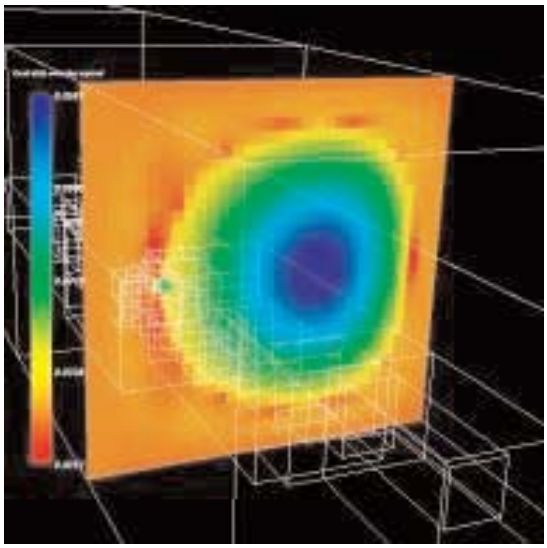


FIGURE 1. AMR simulation of a fuel pellet being injected into a tokamak. Image shows the pressure along a slice as well as the outlines of the various refined grid patches (in collaboration with the SciDAC CEMM project).

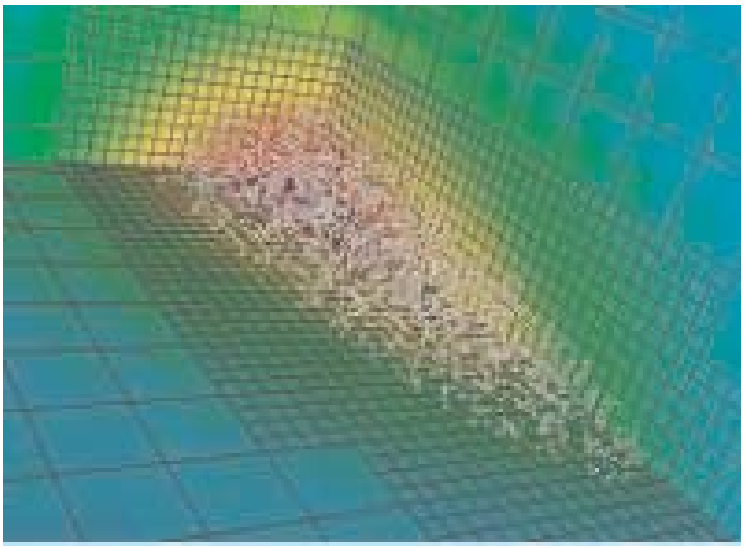


FIGURE 2. AMR particle-in-cell calculation, showing the electrostatic field induced by the particles (in collaboration with the SciDAC AST project).

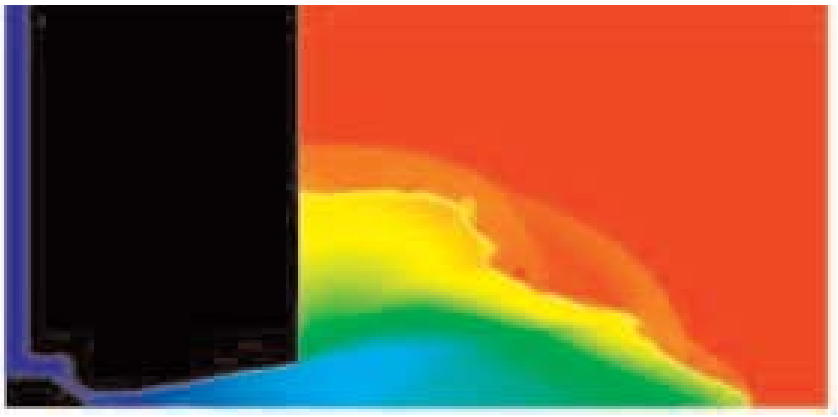


FIGURE 3. Axisymmetric gas jet expanding into a vacuum, with the axis of symmetry along the bottom of the figure, in a laser-driven plasma-wakefield accelerator (in collaboration with the SciDAC AST project).

problems in jets and capillary tubes arising in the design of plasma-wakefield accelerators (Figure 3).

To manage these and other complex AMR algorithms and software, the APDEC team used a collection of libraries written in a combination of programming languages. This software architecture, which maps the mathematical structure of the algorithm space onto a hierarchy of software layers, enables the codes to be more easily adapted and reused across multiple applications. The project team has also developed new grid-generation tools for calculations using mathematical representations from microscopy, medical image data and geophysical data.

Since the APDEC was established, a guiding principle has been to develop a software infrastructure that performs as efficiently as possible. By creating algorithms to efficiently use the number of available processors and combining these with tools for load balancing, the result is software which has a computational cost per grid point and scalability comparable to that of uniform-grid calculations using the same algorithms, giving scientists more detailed results without requiring additional computing resources.

For AMR algorithms for simple compressible flow models, the APDEC project has measured 75 percent efficiency up to 1,024 processors on IBM SP and HP Alpha systems. For incompressible flow, they have observed 75 percent efficiency up to 256 processors. For low-Mach-number combustion, production calculations on IBM SP and SGI systems are typically done using 128–512 processors, and the efficiency of the APDEC algorithms has enabled significant scientific achievements in combustion and astrophysics problems.

For many problems, such as combustion applications, a principal barrier to scaling past a few hundred processors is the performance of iterative methods for solving elliptic equations. To address this problem, the APDEC Center is developing a new class of AMR solvers in three dimensions. The goal is to create a solver with a far lower communications-to-computation ratio than traditional iterative methods, which means the solution can be calculated much more quickly. A preliminary implementation of this algorithm has obtained 85 percent efficiency on 1,024 processors, with less than 4 percent of the execution time spent in communications. The APDEC adaptive calculation used 3 billion grid points, as compared to the 2 trillion grid points that would have been required using a uniform grid algorithm at the same resolution, leading to a reduction in computing time of at least two orders of magnitude. This solver is the basis for the AMR-PIC method developed for the beam dynamics codes mentioned above.

Principal Investigator: Phil Colella, Lawrence Berkeley National Laboratory

Terascale Optimal PDE Solvers (TOPS) ISIC

In many areas of science, physical experimentation is impossible, such as with cosmology; dangerous, as with manipulating the climate; or simply expensive, as with fusion reactor design. Large-scale simulations, validated by comparison with related experiments in well-understood laboratory contexts, are used by scientists to gain insight and confirmation of existing theories in such areas, without benefit of full experimental verification. But today's high-end computers, such as those at DOE's supercomputing centers, are one-of-a-kind, and come without all of the scientific software libraries that scientists expect to find on desktop workstations.

The **Terascale Optimal PDE Solvers (TOPS) ISIC** was created to develop and implement algo-

FIGURE 4. Model of the ILC low-loss cavity

rithms and support scientific investigations performed by DOE-sponsored researchers. These simulations often involve the solution of partial differential equations (PDEs) on terascale computers. The TOPS Center researched, developed and deployed an integrated toolkit of open-source, optimal complexity solvers for the nonlinear partial differential equations that arise in many DOE application areas, including fusion, accelerator design, global climate change and reactive chemistry. The algorithms created as part of this project were also designed to reduce current computational bottlenecks by orders of magnitude on terascale computers, enabling scientific simulation on a scale heretofore impossible.

Nonlinear PDEs give mathematical expression to many core DOE mission applications. PDE simulation codes require implicit solvers for the *multirate, multiscale, multicomponent, multiphysics* phenomena of hydrodynamics, electromagnetism, chemical reaction and radiation transport. Currently, such problems typically reach into the tens of millions of unknowns – and this size is expected to increase 100-fold in just a few years.

Unfortunately, the algorithms traditionally used to solve PDEs were designed to address smaller problems and become much less efficient as the size of the system being studied increases. This creates a double jeopardy for applications, particularly in the case when the algorithms are based on iterations – as it takes more computing resources to solve each step of the problem, and the number of steps also goes up. Fortunately, the physical origin of PDE problems often allows them to be addressed by using a sequence of approximations, each of which is smaller than the one before. The solutions to the approximations, which may be obtained more efficiently, are combined judiciously to provide the solution to the original problems. One well-known example of this approach is called the multigrid method, which solves a problem by tackling a coarse approximation and then using the solution to generate the solution of a better approximation, and so on. It can be shown that the performance of multigrid method is optimal for certain classes of problems. The underlying philosophy of this and other similar approaches is to make the majority of progress towards a high quality result through less complex intermediate steps.

The efforts defined for TOPS and its collaborations with other projects have been chosen to revolutionize large-scale simulation through incorporation of existing and new optimal algorithms and code interoperability. TOPS provides support for the software packages Hypre, PARPACK, PETSc, ScaLAPACK, Sundials, SuperLU and TAO, some of which are in the hands of thousands of users, who have created a valuable experience base on thousands of different computer systems.

Software developed and supported by the TOPS project is being used by scientists around the globe. In the past few years, researchers outside the SciDAC community authored more than two dozen scientific papers reporting results achieved using TOPS software. The papers cover many disciplines, from astronomy to chemistry to materials science to nanotechnology to optics.

TOPS solver software has also been incorporated into numerous other packages, some commercial and some freely available. Among the widely distributed packages maintained outside of the SciDAC program that employ or interface to TOPS software "under the hood" are Dspice, EMSolve, FEMLAB, FIDAP, Global Arrays, HP Mathematical Library, libMesh, Magpar, Mathematica, NIKE, Prometheus, SCIRun, SLEPc, Snark and Trilinos.

Finally, TOPS software is taught in many courses in the U.S. and abroad, and forms a core of the annual training workshop sponsored by DOE to introduce researchers to the Advanced CompuTational Software (ACTS) Collection. TOPS software is also regularly featured in short courses at professional meetings.

Principal Investigator: David Keyes, Cornell University

The Terascale Simulation Tools and Technology (TSTT) Center

Terascale computing provides an unprecedented opportunity to achieve numerical simulations at levels of detail and accuracy previously unattainable. DOE scientists in many different application areas can reach new levels of understanding through the use of high-fidelity calculations based on multiple coupled physical processes and multiple interacting physical scales. The best way to achieve detailed and accurate simulations in many application areas, and frequently the only way to obtain useful answers, is to use adaptive, composite, hybrid approaches. However, the best strategy for a particular simulation is not always clear and the only way to find the best method is to experiment with various options. This is both time-consuming and difficult due to the lack of easy-to-apply, interoperable meshing, discretization and adaptive technologies.

The **Terascale Simulation Tools and Technologies (TSTT) Center** was established to address the technical and human barriers preventing the effective use of powerful adaptive, composite, and hybrid methods. The primary objective was to develop technologies that enable application scientists to easily use multiple mesh and discretization strategies within a single simulation on terascale computers. A key aspect of the project is to develop

services that can be used interoperably to enable mesh generation for representing complex and possibly evolving domains, high-order discretization techniques for improved numerical solutions, and adaptive strategies for automatically optimizing the mesh to follow moving fronts or to capture important solution features.

The center encapsulated its research into software components with well-defined interfaces that enable different mesh types, discretization strategies and adaptive techniques to interoperate in a "plug and play" fashion. All software was designed for terascale computing environments with particular emphasis on scalable algorithms for hybrid, adaptive computations and single processor performance optimization.

To ensure the relevance of the project's research and software developments to the SciDAC goals, the TSTT team collaborated closely with both SciDAC application researchers and other ISICs. Specifically, TSTT technologies were integrated into fusion, accelerator design, climate modeling and biology applications to both provide near-term benefits for those efforts as well as receive the feedback for further improvements.

Working with the Accelerator Modeling project, TSTT researchers generated high-quality meshes from CAD (computer-aided design) models for accurate modeling of the interaction region of the PEP II accelerator. This led to the first successful simulation with a transit beam, using the Tau3P accelerator modeling application. This success led to a decision to continue to use Tau3P for PEP-II computations for reaching higher luminosities. Similar mesh generation efforts by TSTT researchers were used to analyze the wakefield in the advanced Damped Detuned Structure and verify important performance characteristics of the system.

TSTT also partnered with SLAC and the TOPS ISIC to create an automatic design optimization loop to provide automatic tuning of accelerator geometries to significantly increase the speed and decrease the cost by which new accelerators can be designed.

In the field of plasma physics, TSTT researchers helped the Center for Extended MHD Modeling (CEMM) solve a number of problems, particularly the case of anisotropic diffusion, after determining that using fewer higher-order elements significantly decreased the total solution time needed to obtain a given accuracy. This demonstration resulted in a new effort by scientists at Princeton Plasma Physics Laboratory (PPPL) to develop fifth-order finite elements for their primary application code, M3D. TSTT researchers also worked with scientists at PPPL to insert adaptive mesh refinement technologies and error estimators directly into the new high-order M3D code.

TSTT researchers are collaborating with climate modeling scientists to develop enhanced mesh generation and discretization capabilities for anisotropic planar and geodesic surface meshes. The initial mesh is adapted and optimized to capture land surface orographic or topographic height fields. This technology has improved the predication of rainfall, snowfall and cloud cover in regional weather models in prototype simulations.

TSTT researchers are collaborating with computational biologists to develop the Virtual Microbial Cell Simulator (VMCS), which is targeting DOE bioremediation problems to clean up heavy metal waste using microbes. Methods developed by TSTT were used to study how microbe communities aggregate in certain environments, providing new insight into the behavior of these microbes.

In partnership with combustion scientists, TSTT researchers have developed a new tool that combines adaptive mesh refinement with front tracking and used this technology to develop a new capability for diesel engine design. This effort has emphasized the modeling of the instability and breakup of a diesel jet into spray, thought to be the first such effort to provide a predictive capability in this arena.

Principal Investigators: Jim Glimm, State University of New York – Stony Brook; Lori Freitag Diachin, Lawrence Livermore National Laboratory

Computer Science ISICs

The software infrastructure vision of SciDAC is for a comprehensive, portable, and fully integrated suite of systems software and tools for the effective management and utilization of terascale computational resources by SciDAC applications. The following four Computer Science ISIC activities addressed critical issues in high performance component software technology, large-scale scientific data management, understanding application/architecture relationships for improved sustained performance, and scalable system software tools for improved management and utility of systems with thousands of processors.

Center for Component Technology for Terascale Simulation Software

The **Center for Component Technology for Terascale Simulation Software (CCTTSS)** was created to help accelerate computational science by bringing a "plug and play" style of programming to high performance computing. Through a programming model called the Common Component Architecture (CCA), scientists can dramatically reduce the time and effort required to compose independently created software libraries

into new terascale applications. This approach has already been adopted by researchers in the application areas of combustion, quantum chemistry and climate modeling, with new efforts beginning in fusion and nanoscale simulations.

While the CCA approach has been more common in industry, the goal of the CCTTSS was to bring a similar approach to scientific computing. Unlike more narrowly focused commercial applications, the scientific CCA effort faced such challenges as maintaining high performance, working with a broad spectrum of scientific programming languages and computer architectures, and preserving DOE investments in legacy codes.

An example of the CCA approach in action is a prototype application being developed within the Community Climate System Model (CCSM) project. The CCA is used at the level of system integration to connect skeleton components for the atmosphere, ocean, sea ice, land surface, river routing, and flux coupler. Prototype applications within the Earth System Modeling Framework (ESMF), the infrastructure targeted for the future CCSM, also employ the CCA, including reusable components for visualization and connectivity.

In addition, CCTTSS researchers are collaborating closely with application scientists to create high-performance simulations in quantum chemistry and combustion. Moreover, new externally funded projects incorporate CCA concepts in applications involving nanotechnology, fusion, and underground transport modeling, and proposals have been recently submitted involving biotechnology and fusion.

As a part of its mission, the CCTTSS has developed production components that are used in scientific applications as well as prototype components that aid in teaching CCA concepts. These freely available components include various service capabilities, tools for mesh management, discretization, linear algebra, integration, optimization, parallel data description, parallel data redistribution, visualization, and performance evaluation. The CCTTSS is also collaborating with the APDEC, TSTT and TOPS SciDAC centers to define common interfaces for mesh-based scientific data management as well as linear, nonlinear, and optimization solvers.

SciDAC funding has accelerated both CCA technology development and the insertion of this technology into massively parallel scientific applications, including major SciDAC applications in quantum chemistry and combustion. Additionally, numerous CCA-compliant application components have been developed and deployed, and the underlying infrastructure is maturing and establishing itself in the scientific community.

Principal Investigator: Rob Armstrong, Sandia National Laboratories

High-End Computer System Performance: Science and Engineering ISIC

As supercomputers become ever more powerful tools of scientific discovery, demand for access to such resources also increases. As a result, many scientists receive less time on supercomputers than they would like. Therefore, it's critical that they make the most of their time allocations. One way to achieve this optimal efficiency is to analyze the performance of both scientific codes and the computer architectures on which the codes are run. The resulting improvements can be dramatic. In one instance, an astrophysics code which had been running at about 10 percent of a supercomputer's theoretical peak speed (which is typical) was able to run at more than 50 percent efficiency after careful performance analysis and tuning.

SciDAC's **High-End Computer System Performance: Science and Engineering ISIC**, also known as the Performance ISIC or PERC, focused on developing tools and techniques to help scientists determine how they can best execute a specific application on a given computer platform. The research was aimed at determining what level of achievable performance is realistic, how scientific applications can be accelerated toward these levels, and how this information can drive the design of future applications and high-performance computing systems.

In addition to helping scientists better understand performance behavior of their codes, the major improvements to computer performance modeling technology made by PERC researchers are also helping supercomputer centers to better select systems, thereby ensuring higher scientific productivity on these publicly funded systems. Such supercomputer procurements run to millions of dollars, and PERC research is being used by centers operated by DOE, the National Science Foundation and the Department of Defense around the country. PERC researchers have also collaborated with several SciDAC scientific application efforts, resulting is major speedups for several high-profile computer codes used in these projects.

For the **Community Climate System Model (CCSM)**, one of the United States' primary applications for studying climate change, PERC researchers helped determine optimal algorithmic settings for the Community Atmosphere Model (CAM), a key component of the CCSM, when running the Intergovernmental Panel on Climate Change scenario runs on the IBM p690 cluster computer at ORNL, accelerating the completion of this milestone. Similar studies are ongoing on the SGI Altix, Cray XD1, and Cray XT3 supercomputers. The resulting data from these runs will contribute to an international report on global climate change.

Working with the **Plasma Microturbulence Project (PMP),** PERC researchers applied Active Harmony, a software tool supporting distributed execution of computational objects, to GS2, a gyrokinetic turbulence simulator used by the fusion energy research community. The result was a 2.3 to 3.4 times speedup of GS2 for a common configuration used in production runs.

PERC researchers worked with the **Terascale Supernovae Initiative (TSI)** project to port and optimize the EVH1 hydrodynamics code on the Cray X1 supercomputer, achieving excellent performance for large problems. The EVH1 performance analysis was completed for up to 256 processors on all current target platforms.

Working with two other ISICs, the **Terascale PDE Simulations (TOPS) and Terascale Simulation Tools and Technology (TSTT)** centers, PERC researchers analyzed the performance of a TOPS-TSTT mesh smoothing application and found that the sparse matrix-vector multiply achieves 90 percent of the peak performance imposed by the memory bandwidth limit.

PERC researchers collaborated closely with SciDAC's **Lattice Gauge Theory** project, conducting performance analyses of the MILC (MIMD Lattice Computation) application on Pentium-3 Linux clusters. The PERC team collected detailed performance data on different aspects of the code and identified the key fragments that affect the code performance, then presented their findings to the lattice gauge theory community.

In the **Accelerator Science and Technology** program, the PERC team has shown how to improve the performance of the post-processing phase within the Omega3P application at the Stanford Linear Accelerator Center. Post-processing can consume 40 percent or more of total execution time in a full run of Omega3P, where most of this time is due to a complex and redundant computation. By exchanging this redundant computation for cached lookup to pre-computed data, researchers were able to achieve 4.5 times speedups of the post-processing phase, and 1.5 time speedups of a full Omega3P run.

In addition to working directly with scientists on the performance of codes, PERC researchers have made major improvements in the usability and effectiveness of several performance tools, enabling researchers to analyze their codes more easily. The result is an integrated suite of measurement, analysis and optimization tools to simplify the collection and analysis of performance data and help users in optimizing their codes.

Principal Investigator: David Bailey, Lawrence Berkeley National Laboratory

Scalable Systems Software for Terascale Computer Centers

As terascale supercomputers become the standard environment for scientific computing, the nation's premiere scientific computing centers are at a crossroads. Having built the operations of their systems around home-grown systems software, system administrators and managers now face the prospect of rewriting their software, as these incompatible, ad hoc sets of systems tools were not designed to scale to the multi-teraflop systems that are being installed in these centers today. One solution would be for each computer center to take its home-grown software and rewrite it to be scalable. But this would incur a tremendous duplication of effort and delay the availability of terascale computers for scientific discovery.

The goal of the SciDAC's **Scalable Systems Software** project is to provide a more timely and cost-effective solution by pulling together representatives from the major computer centers and industry and collectively defining standardized interfaces between system components. At the same time, this group is producing a fully integrated suite of systems software components that can be used by the nation's largest scientific computing centers.

The Scalable Systems Software suite is being designed to support computers that scale to very large physical sizes without requiring that the number of support staff scale along with the machine. But this research goes beyond just creating a collection of separate scalable components. By defining a software architecture and the interfaces between system components, the Scalable Systems Software research is creating an interoperable framework for the components. This makes it much easier and cost effective for supercomputer centers to adapt, update, and maintain the components in order to keep up with new hardware and software. A well-defined interface allows a site to replace or customize individual components as needed. Defining the interfaces between components across the entire system software architecture provides an integrating force between the system components as a whole and improves the long-term usability and manageability of terascale systems at supercomputer centers across the country.

The Scalable Systems Software project is a catalyst for fundamentally changing the way future high-end systems software is developed and distributed. The project is expected to reduce facility management costs by reducing the need to support home-grown software while making higher quality systems tools available. The project will also facilitate more effective use of machines by scientific applications by providing scalable job launch, standardized job monitoring and management software, and allocation tools for the cost-effective management and utilization of terascale and petascale computer resources.

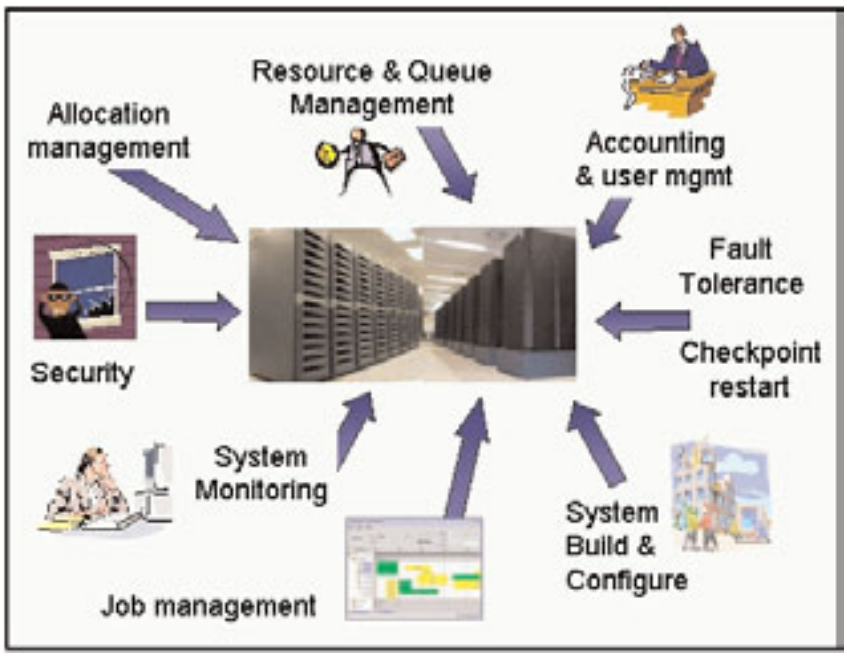


FIGURE 5. The mission of the Scalable Systems Software center is the development of an integrated suite of systems software and tools for the effective management and utilization of terascale computational resources, particularly those at the DOE facilities.

Here are some of the highlights of the project:

Designed modular architecture: A critical component of the project's software design is its modularity. The ability to plug and play components is important because of the diversity in both high-end systems and the individual site management policies.

Defined XML-based interfaces that are independent of language and wire protocol: The interfaces between all the components have been fully documented and made publicly available, thereby allowing others to write replacement components (or wrap their existing components) as needed. The reference implementation has a mixture of components written in a variety of common programming languages, which allows a great deal of flexibility to the component author and allows the same interface to work on a wide range of hardware architectures and facility polices.

Reference implementation released: Version 1.0 of the fully integrated systems software suite was released at the SC2005 conference – the leading international meeting of the supercomputing community – and will be followed by quarterly updates for the following year.

Production users: Full system software suites have been put into production on clusters at Ames Laboratory and Argonne National Laboratory. Pacific Northwest National Laboratory and the National Center for Supercomputer Applications have adopted one or more components from the suite, and the project team is in discussion with Department of Defense sites about use of some of the system software components.

Adoption of application programming interface (API): The suite's scheduler component is the widely used Maui Scheduler. The public Maui release (as well as the commercial Moab scheduler) has been updated to use the public XML interfaces and has added new capabilities for fairness, higher system utilization, and improved response time. All new Maui and Moab installations worldwide (more than 3,000/month) now use the system software interfaces developed in this ISIC. Prominent users include 75 of the world's top 100 supercomputers and commercial industries such as Amazon.com and Ford Motor Co.

Principal Investigator: Al Geist, Oak Ridge National Laboratory

The Scientific Data Management Center

Scientific exploration and discovery typically takes place in two phases: generating or collecting data and then analyzing the data. In the data collection/generation phase, large volumes of data are generated by simulation programs running on supercomputers or collected from experiments. As experimental facilities and computers have become larger and more powerful, the amount of resulting data threatens to overwhelm scientists. Without effective tools for data collection and analysis, scientists can find themselves spending more time on data management than on scientific discovery.

The **Scientific Data Management Center (SDM)** was established to focus on the application of known and emerging data management technologies to scientific applications. The center's goals are to integrate and deploy software-based solutions to the efficient and effective management of large volumes of data generated by scientific applications. The purpose is not only to achieve efficient storage and access to the data using specialized indexing, compression, and parallel storage and access technology, but also to enhance the effective use of the scientists' time by eliminating unproductive simulations, by providing specialized data-mining techniques, by streamlining time-consuming tasks, and by automating the scientists' workflows.

The center's approach is to provide an integrated scientific data

management framework where components can be chosen by scientists and applied to their specific domains. By overcoming the data management bottlenecks and unnecessary information-technology overhead through the use of this integrated framework, scientists are freed to concentrate on their science and achieve new scientific insights.

Today's computer simulations and large-scale experiments can generate data at the terabyte level, equivalent to about 5 percent of all the books in the Library of Congress. Keeping up with such a torrent of data equires efficient parallel data systems. In order to make use of such amounts of data, it is necessary to have efficient indexes and effective analysis tools to find and focus on the information that can be extracted from the data, and the knowledge learned from that information. Because of the large volume of data, it is also useful to perform analysis as the data are generated. For example, a scientist running a thousand-time-step, 3D simulation can benefit from analyzing the data generated by the individual steps in order to steer the simulation, saving unnecessary computation, and accelerating the discovery process. However, this requires sophisticated workflow tools, as well as efficient dataflow capabilities to move large volumes of data between the analysis components. To enable this, the center uses an integrated framework that provides a scientific workflow capability, supports data mining and analysis tools, and accelerates storage access and data searching. This framework facilitates hiding the details of the underlying parallel and indexing technology, and streamlining the assembly of modules using process automation technologies.

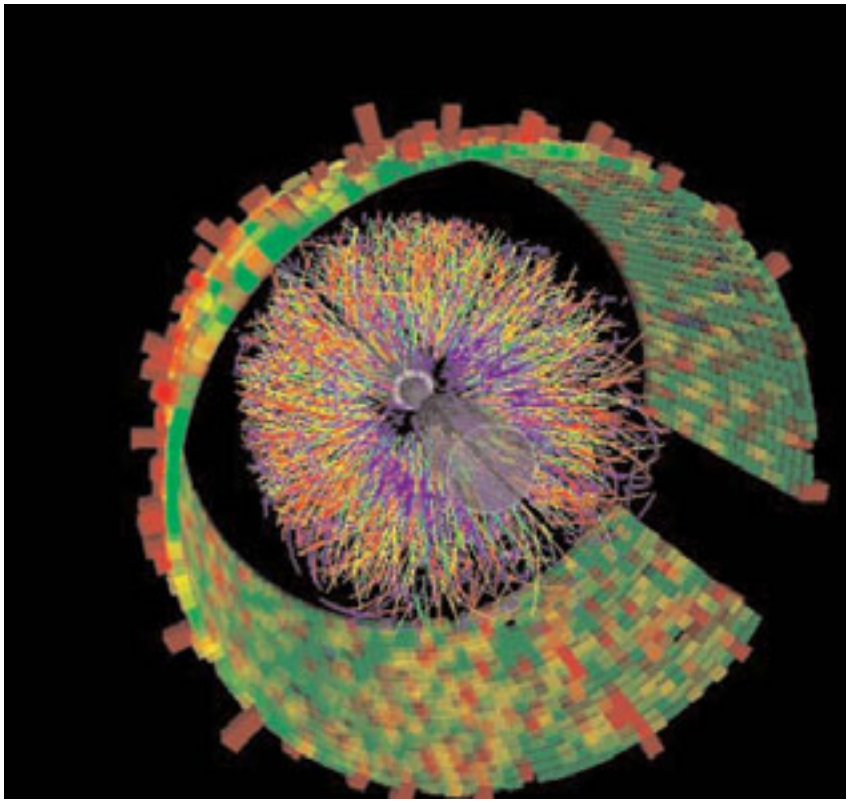


FIGURE 6. The STAR Experiment at Brookhaven National Laboratory generates petabytes of data resulting from the collisions of millions of particles. The Scientific Data Management ISIC developed software to make it easier for scientists to transfer, search and analyze the data from such large-scale experiments.

Since it was established, SDM has adopted, improved and applied various data management technologies to several scientific application areas. By working with scientists, the SDM team not only learned the important aspects of the data management problems from the scientists' point of view, but also provided solutions that led to actual results. The successful results achieved so far include:

- More than a tenfold speedup in writing and reading NetCDF files was achieved by developing Parallel NetCDF software on top of the MPI-IO.
- An improved version of PVFS is now offered by cluster vendors, including Dell, HP, Atipa, and Cray.
- A method for the correct classification of orbits in puncture plots from the National Compact Stellarator eXperiment (NCSX) at PPPL was developed by converting the data into polar coordinates and fitting second-order polynomials to the data points.
- A new specialized method for indexing using bitmaps was used to provide flexible efficient search over billions of collisions (events) in high energy physics applications. A paper on the system received best paper award at the 2004 International Supercomputing Conference.
- The development of a parallel version of the popular statistical package R is being applied to fusion, geographic information systems and proteomics (biochemistry) applications.
- A scientific workflow system was developed and applied to the analysis of microarray data, as well as astrophysics applications. The system greatly increased the efficiency of running repetitive processes.

Principal Investigator: Arie Shoshani, Lawrence Berkeley National Laboratory

Creating an Advanced Infrastructure for Increased Collaboration

A hallmark of many DOE research efforts is collaboration among scientists from different disciplines. The multidisciplinary approach is the driving force behind the "big science" breakthroughs achieved at DOE national laboratories and other research institutions. By creating teams comprising physicists, chemists, engineers, applied mathematicians, biologists, earth scientists, computer scientists and others, even the most challenging scientific problems can be defined, analyzed and addressed more effectively than if tackled by one or two scientists working on their own.

With the advent of high-performance computers and networks, such teams can now be assembled virtually, with a multitude of research talents brought to bear on scientific problems of national and global importance. DOE scientists and engineers have been developing technologies in support of these "collaboratories." The goal is to make collaboration among scientists at geographically dispersed sites as effective as if they were working at the same location. A key aspect of collaboratories is providing seamless and secure access to experimental facilities and computing resources at sites around the country.

As these collaborative experiments, whether a particle accelerator in New York or a massive telescope atop a volcano in Hawaii, come on line, scientists will be inundated with massive amounts of data which must be shared, analyzed, archived and retrieved by multiple users from multiple sites. Large research programs are producing data libraries at the petabyte level, the equivalent of 500 billion standard-size document pages, or 100 times the data volume of the U.S. Library of Congress. Tools which enable the easy transfer of huge datasets are essential to the success of these research efforts.

Under SciDAC, a number of collaboratory infrastructure projects were established to advance collaborative research. These projects incorporated technologies from distributed systems often referred to as "Grids." Built upon networks like the Internet, a computing Grid is a service for sharing computer power and data storage capacity over the Internet, resulting in large, distributed computational resources. DOE is expanding the concept of Grids beyond computers to integrate access to experimental facilities and data archives around the world. While the idea is straightforward, developing a unified, secure infrastructure linking various systems with unique security and access procedures, sometimes across international boundaries, is a daunting task.

Grid technology is evolving to provide the services and infrastructure needed for building "virtual" systems and organizations. A Grid-based infrastructure provides a way to use and manage widely distributed computing and data resources to support science. The result is a standard, large-scale computing, data, instrument, and collaboration environment for science that spans many different projects, institutions, and countries.

National Collaboratory Projects

DOE's investment in National Collaboratories includes four SciDAC projects focused on the goal of creating collaboratory software environments to enable geographically separated scientists to effectively work together as a team and to facilitate remote access to both facilities and data.

The DOE Science Grid

A significant portion of DOE science is already, or is rapidly becoming, a distributed endeavor involving many collaborators who are frequently working at institutions across the country or around the world. Such collaborations typically have rapidly increasing needs for high-speed data transfer and high-performance computing. More and more, these requirements must be addressed with computing, data,

and instrument resources that are often more widely distributed than the collaborators. Therefore, developing an infrastructure that supports widely distributed computing and data resources is critical to DOE's leading-edge science.

Such infrastructures have become known as Grids, which provide secure and reliable access to these critical resources. While the individual institutions have their own policies and procedures for providing access to users, successful deployment of a Grid requires that a common approach be implemented so that when an authorized user logs into a Grid, all appropriate resources can be easily accessed.

Under SciDAC, the DOE Science Grid was developed and deployed across the DOE research complex to provide persistent Grid services to advanced scientific applications and problem-solving frameworks. By reducing barriers to the use of remote resources, it has made significant contributions to SciDAC and the infrastructure required for the next generation of science. The DOE Science Grid testbed was initially deployed among five project sites: the National Energy Research Scientific Computing Center and Argonne, Lawrence Berkeley, Oak Ridge and Pacific Northwest national laboratories.

In addition to the construction of a Grid across five major DOE facilities with an initial complement of computing and data resources, other accomplishments include:

- Integration into the Grid of the large-scale computing and data storage systems at NERSC, DOE's Office of Science flagship supercomputing center.
- Design and deployment of a Grid security infrastructure that is facilitating collaboration between U.S. and European high energy physics projects, and within the U.S. magnetic fusion community. This infrastructure provides a global, policy-based method of identifying and authenticating users, which leads to a "single sign-on" so that any system on the Grid can accept a uniform user identity for authorization. This work is currently used by DOE's Particle Physics Data Grid, Earth Systems Grid, and Fusion Grid projects.
- A resource monitoring and debugging infrastructure that facilitates managing this widely distributed system and the building of high performance distributed science applications.
- Development and deployment partnerships established with several key vendors.
- Use of the Grid infrastructure by applications from several disciplines – computational chemistry, groundwater transport, climate modeling, bioinformatics, etc.
- In collaboration with DOE's Energy Sciences Network (ESnet), the design and deployment of the DOE Grids Certification Authority (Grid authentication infrastructure) that provides Grid identity certificates to users, systems, and services, based on a common, science collaboration oriented policy that is defined and administered by the subscribing virtual organizations.

Principal Investigator: William Johnston, Lawrence Berkeley National Laboratory

The National Fusion Collaboratory

Developing a reliable energy system that is economically and environmentally sustainable is the long-term goal of DOE's Fusion Energy Science (FES) research program. In the U.S., FES experimental research is centered at three large facilities with a replacement value of over $1 billion. As these experiments have increased in size and complexity, there has been a concurrent growth in the number and importance of collaborations among large groups at the experimental sites and smaller groups located nationwide.

The next generation fusion experimental device is the ITER reactor, an international collaboration with researchers from China, Europe, India, Japan, Korea, Russia and the U.S. ITER will be a burning fusion plasma magnetic confinement experiment located in France. With ITER located outside the U.S., the ability to maximize its value to the U.S. program is closely linked to the development and deployment of collaborative technology. As a result of the highly collaborative present and future nature of FES research, the community is facing new and unique challenges.

The **National Fusion Collaboratory** established under SciDAC unites fusion and computer science researchers to directly address these challenges by creating and deploying collaborative software tools. In particular, the project has developed and deployed a national FES Grid (FusionGrid) that is a system for secure sharing of computation, visualization and data resources over the Internet. This represents a fundamental paradigm shift for the fusion community where data, analysis and simulation codes, and

FIGURE 1. The control rooms of NSTX (a), DIII-D (b), and C-Mod (c) with shared display walls being used to enhance collocated collaboration. On the DIII-D shared display is also video from remote collaborators in Europe who were participating in that day's experiment.

FIGURE 2. FusionGrid services are being used to collaborate in real time by fusion scientists in the U.S. and abroad. Pictured in the foreground is Dr. deGrassie (San Diego) leading the JET experiment (England), and on the screen is the JET control room and various JET data traces being discussed in real time.

visualization tools are now thought of as network services. In this new paradigm, access to resources (data, codes, visualization tools) is separated from their implementation, freeing the researcher from needing to know about software implementation details and allowing a sharper focus on the physics. The long-term goal of FusionGrid is to allow scientists at remote sites to participate as fully in experiments and computational activities as if they were working on site, thereby creating a unified virtual organization of the geographically dispersed U.S. magnetic fusion community – more than 1,000 researchers from over 40 institutions.

Fusion scientists use the FusionGrid to provide wide access to the complex physics codes and associated data used for simulating and analyzing magnetic fusion experiments. The first FusionGrid service came online in fall 2002. Since then, the service – a transport code known as TRANSP – has been used by scientists to produce over 6,000 code runs and has supported analysis of fusion devices on three continents. TRANSP was also used to demonstrate the feasibility of between-shot analysis on FusionGrid.

Fusion scientists also use the FusionGrid as an advanced collaborative environment service that provides computer-mediated communications techniques to enhance work environments and to enable increased productivity for collaborative work. In January 2004 a fusion scientist in San Diego remotely led an experiment on the largest European magnetic fusion experiment, located in the United Kingdom, using FusionGrid's remote collaboration services. These services included multiple video images and a unified audio stream along with real-time secure access to data. With the introduction of FusionGrid's remote collaboration services, remote participation in fusion experiments is becoming more commonplace.

The National Fusion Collaboratory project is also working to enhance collaboration within the control rooms of fusion experiments. Shared display walls have been installed in the control rooms of the three large U.S. fusion experiments for enhanced large-group collaboration. The project has created and deployed unique software that presents the scientists with a multi-user environment allowing them to simultaneously share data to the large display and simultaneously interact with the display to edit, arrange, and highlight information. For collocated scientists, the ability to publish and share a scientific graph on the display wall results in easier and broader discussion compared to the old model of a few individuals gathering around a small computer monitor. For remote scientists, the ability of the shared display to accept video combined with audio has allowed them to interact and even lead an experiment.

Taken as a whole, the technologies being deployed by the National Fusion Collaboratory project are further facilitating data sharing and decision-making by both collocated and remote scientists. With the eyes of the worldwide fusion community shifting towards France for the next generation device, ITER, such capability becomes increasingly important for scientific success.

Principal Investigator: David Schissel, General Atomics

The Particle Physics Data Grid

The Department of Energy's national laboratories are home to some of the world's leading facilities for particle physics experiments. Such experiments typically generate millions of particles which must be extensively analyzed and filtered to find and measure the exotic particles that herald new discoveries. The **Particle Physics Data Grid** (PPDG) collaboratory was launched as a collaboration between physicists and computer scientists to adapt and extend Grid technologies and the physicists' applications to build distributed systems to handle the storage, retrieval and analysis of the particle physics data at DOE's most critical research facilities.

PPDG has been instrumental in the significant progress made over the past five years in deploying Grid-enabled, end-to-end capabilities into the production data processing infrastructure of the participating experiments, and in making extended and robust Grid technologies generally available. Also, PPDG has successfully demonstrated the effectiveness of close collaboration between end users and the developers of new distributed technologies.

The experiments involved span those already in steady data-taking mode – where existing production systems were carefully extended step by step to take advantage of Grid technologies – to those developing new global systems for detector commissioning and the acquisition of data.

As a result of PPDG and other Grid projects in the U.S. and Europe, particle physics collaborations now include Grid-distributed computing as an integral part of their data processing models. By collaboratively deploying their developed technologies into significant production use, the computer science groups have extended their technologies and made them generally available to benefit other research communities.

In addition to the experiment-specific end-to-end systems, through partnering with the National Science Foundation's iVDGL and GriPhyN projects and working with European counterparts such as the European Data Grid and Enabling Grids for EsciencE, PPDG has helped pave the way for a worldwide multi-science production Grid infrastructure. In the U.S., PPDG has played a leadership role in creating first the Grid3 and now the Open Science Grid infrastructure, which provides a common software installation, operational procedures and sharing of services for 50 laboratory and university sites.

The PPDG-supported improvements in data handling include a tenfold increase in the amount of sustained data distribution, a 50 percent reduction in the effort required to distribute data and analysis among five institutions, and up to a 50 percent increase in available resources due to Grid-enabled sharing. And even though funding for the PPDG has concluded, the collaborations established under the program continue to boost scientific productivity.

Significant scientific results and benefits that the technology developments and collaborations in PPDG have enabled include:

- The shortened turnaround time for analysis of the STAR nuclear physics experiment data produced early results in the first direct measurement of particles known as "open charm" production at the Relativistic Heavy Ion Collider. This was enabled through the experiment's collaboration with the Storage Resource Management group, which for the past few years has provided sustained transfer of more than 5 terabytes a week between Brookhaven National Laboratory in New York and Lawrence Berkeley National Laboratory in California.
- All results from the Fermilab Tevatron experiments, CDF and D0, now rely on distributed computing using Grid technologies. Up to 20 sites around the world now receive and analyze data from the D0 experiment, which has led to new discoveries, such as results showing the mixing of B_s mesons, mesons that contain a "beauty quark" and a "strange quark." The PPDG has contributed to such successes by improving a number of the software applications used to transfer and analyze data, more than doubling the efficiency of these operations. CDF seamlessly supports simulation and analysis jobs at up to 10 sites in Europe and the U.S.
- The BaBar experiment at the Stanford Linear Accelerator Center routinely moves all the data collected from the accelerator to computing centers in France, Italy and England. The Storage Resource Broker was extended to provide the distributed catalogs describing and managing the data. These catalogs are necessary to manage the location and selection information for the multipetabyte distributed datasets.
- The Large Hadron Collider (LHC) experiments are participating in a worldwide Grid project to provide global distribution and analysis of data from CERN in Switzerland. The U.S. ATLAS and U.S. CMS collaborations are developing and testing their physics algorithms and distributed infrastructure in preparation for the onslaught of tens of petabytes a year of data to be analyzed by 2008. At the end of 2005, ATLAS produced more than one million fully simulated events on the Open Science Grid with 20 different physics samples to test the data distribution and analysis capabilities. CMS is running "Data Challenges" to distribute data from the CERN accelerator location to the global sites. Data is transferred from

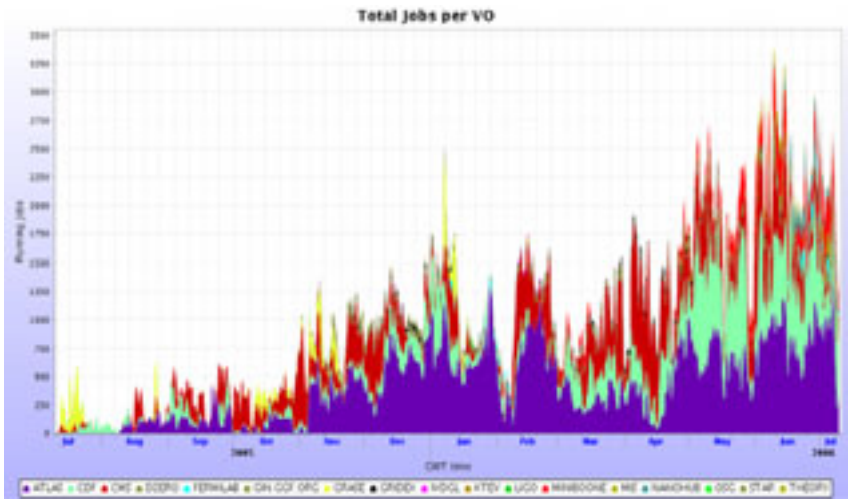


FIGURE 3: Monitored Jobs on Open Science Grid

the U.S. Tier-1 Center to sites around the world as part of the data distribution and analysis system. Peak transfer rates of ~5 Gbps are reached.

- The Open Science Grid Consortium provides a common infrastructure, validated software stack and ongoing operations and collaboration which all the groups in PPDG use and to which PPDG has made significant contributions. The use of Open Science Grid has increased steadily since its launch in July 2005, and it is hoped to continue with this work to benefit all the PPDG collaborators over the next few years. Ideally, the significant progress made by PPDG towards a usable, global computing infrastructure supporting large institutions can be extended to benefit smaller research programs and institutions as well.

Principal Investigators: Richard Mount, Stanford Linear Accelerator Center; Harvey Newman, California Institute of Technology; Miron Livny, University of Wisconsin Madison; Ruth Pordes, Fermi National Accelerator Laboratory (added 2003).

The Earth System Grid II: Turning Climate Model Datasets into Community Resources

One of the most important – and challenging – scientific problems which requires extensive computational simulations is global climate change. The United States' climate research community has created the Community Climate System Model (CCSM), one of the world's leading climate modeling codes. By changing various conditions, such as the emission levels of greenhouse gases, scientists can model different climate change scenarios. Because running such simulations is computationally demanding, the code is only being run at a few DOE computing facilities and the National Center for Atmospheric Research. The resulting data archive, distributed over several sites, currently contains upwards of 100 terabytes of simulation data and continues to grow to petabytes by the end of the decade. Making the data available to a broad range of researchers for analysis is key to a comprehensive study of climate change.

SciDAC's **Earth System Grid (ESG)** is a collaborative interdisciplinary project aimed at addressing the challenge of enabling management, discovery, access and analysis of these enormous and extremely important data assets. For the modeling teams, the daily management and tracking of their data is already proving to be a significant problem. Then there are climate researchers working at institutions and universities across the U.S. whose ability to discover and use the data is extremely limited. That's today, and the problem is rapidly escalating.

As computers become more powerful and can run the models faster and with more complex details, such as finer geographic resolution, the amount of data will increase significantly. Much of the current modeling activity is focused upon simulations aimed at the upcoming Intergovernmental Panel on Climate Change (IPCC) assessment, and these simulations have twice the horizontal resolution of the models that have been run for the past several years, which increases the resulting data volume fourfold. Figure 4 depicts new work representing yet another doubling of the resolution.

All of this adds up to an enormous increase in the volume and complexity of data that will be produced. Moving that data will become increasingly costly, which could discourage the sharing of data among the community of climate researchers.

The heart of ESG is a simple, elegant, and powerful Web portal that allows scientists to register, search, browse, and acquire the data they need. This portal was demonstrated at the Supercomputing 2003 conference on high performance computing. The portal incorporates new capabilities for cataloging datasets, registering new users and interoperability between different mass storage architectures.

One of ESG's strategies is to dramatically reduce the amount of data that needs to be moved over the network, and the project team

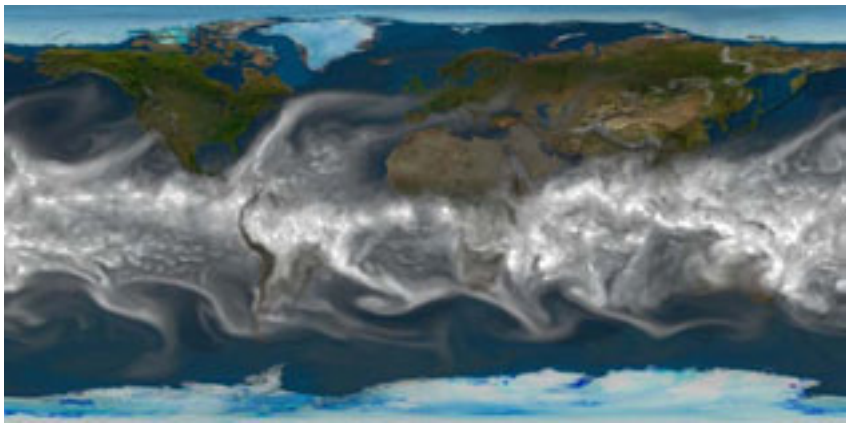


FIGURE 4: From the atmospheric component of the CCSM, this visualization shows precipitable water from a high-resolution experimental simulation (T170 resolution, about 70 km).

has done groundbreaking work in developing generalized remote data access capabilities. This involves heavy collaboration with the SciDAC DataGrid Toolkit project, as well as joint work with the community OpenDAP project.

In summer 2004, ESG began serving IPCC and other model data to a global community in close partnership with the IPCC effort and the World Meteorological Organization.

Principal Investigator: Ian Foster, Argonne National Laboratory

Security and Policy for Group Collaboration

Today, scientific advances are rarely the result of an individual toiling in isolation, but rather the result of collaboration. Such collaborations are using their combined talents to address scientific problems central to DOE's mission in areas such as particle physics experiments, global climate change and fusion science. While considerable work has been done on tools to help perform the work of a collaboration, little attention has been paid to creating mechanisms for establishing and maintaining the structure of such collaborative projects. This structure includes methods for identifying who are members of the collaboration, what roles they play, what types of activities they are entitled to perform, what community resources are available to members of the collaboration and what are the policies set down by the owners of those resources.

The **Security and Policy for Group Collaboration** project was created to develop scalable, secure and usable methods and tools for defining and maintaining membership, rights, and roles in group collaborations. Such collaborations share common characteristics:

- The participants, as well as the resources, are distributed both geographically and organizationally.
- Collaborations can scale in size from a few individuals to thousands of participants, and membership may very dynamic.
- Collaborations may span areas of expertise, with members filling different roles within the collaboration.
- The work of the team is enabled by providing team members with access to a variety of community resources, including computers, storage systems, datasets, applications, and tools.

Central to this problem of structure is determining the identity of both participants and resources and, based on this identity, determining the access rights of the participant and the policy of the resource. While mechanisms for authentication and authorization have been defined, the issues of distribution, dynamics and scale complicate their application to collaborative environments. Additionally, sites providing the resources for a collaboration often have overruling security mechanisms and policies in place which must be taken into account, rather than replaced by the collaboration.

The project team has instantiated its research results into the Globus Toolkit's® widely used Grid Security Infrastructure. Since the Globus Toolkit is already adopted by many science projects – the Particle Physics Data Grid, Earth Systems Grid, DOE Science Grid and other non-DOE Grid activities like NSF TeraGrid, NASA IPG and the European Data Grid – the project's mechanisms for security and authentication can be easily used by these scientists.

Principal Investigator: Stephen Tuecke, Argonne National Laboratory

Middleware Projects

Two projects are conducting research and development that will address individual technology elements to enable universal, ubiquitous, easy access to remote resources and to contribute to the ease with which distributed teams work together. Enabling high performance for scientific applications is especially important.

Middleware Technology to Support Science Portals: Gateways to the Grid

While extensive networks such as the Internet have been in existence for decades, it took the organization of the World Wide Web and the creation of easy-to-use Web browsers to make the Internet the dynamic information resource that

it is today. In much the same way, networked Grids linking computing, data and experimental resources for scientific research have the potential to greatly accelerate collaborative scientific discovery.

Under SciDAC, the **Middleware Technology to Support Science Portals** project was created to develop a "Science Portal" environment which would allow scientists to program, access and execute distributed Grid applications from a conventional Web browser and other tools on their desktop computers. Portals allow each user to configure their own problem-solving environment for managing their work. The goal is to allow the scientist to focus completely on the science by making the Grid a transparent extension of the user's desktop computing environment.

The first step in this project was to create a software platform for building the portal and which could be used as a testbed. Then the project team partnered with applications researchers to get feedback on how well the applications worked when accessed by portal users. For applications, the project partnered with several National Science Foundation (NSF) projects. The team also worked with the Global Grid Forum, with NSF funding, to refine the research portal technology for production use.

Principal Investigator: Dennis Gannon, Indiana University

DataGrid Middleware: Enabling Big Science on Big Data

Many of the most challenging scientific problems being addressed by DOE researchers require access to tremendous quantities of data as well as computational resources. Physicists around the world cooperate in the analysis of petabytes of accelerator data. Climate modelers compare massive climate simulation outputs. Output from multi-million dollar online instruments, such as the Advanced Photon Source or earthquake engineering shake tables, must be visualized in real time so that a scientist can adjust the experiment while it is running.

In order for these applications to be feasible, infrastructure must be in place to support efficient, high performance, reliable, secure, and policy aware management of large-scale data movement. The SciDAC **DataGrid Middleware** project has provided tools in three primary areas in support of this goal. GridFTP, developed primarily at Argonne National Laboratory, provides a secure, robust, high performance transport mechanism that is recognized as the de facto standard for transport on the Grid. The Globus replica tools, developed primarily at the University of Southern California's Information Sciences Institute, provide tracking of replicated data sets and provide efficiency in the selection of data sets to access. The Condor team at the University of Wisconsin is providing storage resource management, particularly space reservation tools. Together, these three components provide the basis for DataGrid applications.

These DataGrid tools are being used by other SciDAC projects. The Earth System Grid and the Particle Physics Data Grid use GridFTP servers to stage input data and move results to mass storage systems. They also employ the project's first generation replica catalog to determine the best location from which to store and/or retrieve data. The Laser Interferometer Gravitational Wave Observatory project has moved over 50 terabytes of data and has a replica location service with over 3 million logical files and over 30 million physical filenames. The Grid3 project, part of the Grid Physics Network, moves over 4 terabytes of data a day. GridFTP is now a Global Grid Forum standard and there is a replication working group working on standards as well. The tools developed as part of this project have become the de facto standard for data management and, in fact, are opening up new realms of scientific discovery.

For example, participants in the Large Hadron Collider experiment, which will come on line in 2007 in Switzerland, are conducting "data challenges" to ensure that the data coming out of the experiment can be accommodated. In a 2005 challenge, a continuous average data flow of 600 megabytes per second was sustained over 10 days, for a total transfer of 500 terabytes of data – all enabled by GridFTP. Moving the same amount of data over a typical household network connection (at 512 kilobits per second) would take about 250 years.

Principal Investigators: Ian Foster, Argonne National Laboratory; Carl Kesselman, University of Southern California Information Sciences Institute; Miron Livny, University of Wisconsin-Madison

Networking Projects

As high-speed computer networks play an increasingly important role in large-scale scientific research, scientists are becoming more dependent on reliable and robust network connections, whether for transferring experimental data, running applications on distributed supercomputers or collaborating across the country or around the globe. But as anyone who has logged onto the Internet can attest, network connections can unexpectedly break or bog down at any time. To help keep such system problems from disrupting scientific research, SciDAC funded three research projects to develop better methods for analyzing and addressing network performance.

INCITE: Monitoring Performance from the Outside Looking In

The **INCITE (InterNet Control and Inference Tools at the Edge)** project was aimed at developing tools and services to improve the performance of applications running on distributed computing systems linked by computational grids. Although such applications are complex and difficult to analyze, knowledge of the internal network traffic conditions and services could optimize the overall performance. Without special-purpose network support (at every router), the only alternative is to indirectly infer dynamic network characteristics from edge-based network measurements. Therefore, this project researched and developed network tools and services for analyzing, modeling, and characterizing high-performance network end-to-end performance based solely on edge-based measurements made at the hosts and routers at the edges of the network, rather than midpoints on the network. Specifically, the goal was to develop multi-scalable on-line tools to characterize and map network performance as a function of space, time, applications, protocols, and services for end-to-end measurement, prediction, and network diagnosis.

Two of the tools developed by the project have been incorporated into a toolkit used to identify performance problems at a number of major networks and research sites. INCITE users include: Globus, SciDAC's Supernova Science Center and Particle Physics Data Grid Pilot, Scientific Workspaces of the Future, TeraGrid, Transpac at Indiana University, San Diego Supercomputing Center, Telecordia, CAIDA, Autopilot, TAU and the European GridLab project.

Principal Investigator: Richard Baraniuk, Rice University

Logistical Networking: A New Approach for Data Delivery

The project for **Optimizing Performance and Enhancing Functionality of Distributed Applications using Logistical Networking** explored the use of a new technique to provide fast, efficient and reliable data delivery to support the high-performance applications used by SciDAC collaborators. Logistical networking (LN) is a new way of synthesizing networking and storage to create a communication infrastructure that provides superior control of data movement and management for distributed applications based on shared network storage. LN software tools allow users to create local storage "depots" or utilize shared storage depots deployed worldwide to easily accomplish long-haul data transfers, temporary storage of large datasets (on the order of terabytes), pre-positioning of data for fast on-demand delivery, and high performance content distribution such as streaming video.

A primary research drive of the project was to work with SciDAC's Terascale Supernova Initiative (TSI) group, which uses LN to share massive datasets at speeds up to 220 Mbps between Oak Ridge National Laboratory (ORNL) in Tennessee and North Carolina State University (NCSU). A new, private LN infrastructure is in place, designed specifically for TSI and other SciDAC projects. Depots at ORNL, San Diego Supercomputing Center, SUNY-Stony Brook and NCSU provide 8 terabytes of storage and form the network's backbone.

The second area of focus is support for SciDAC's fusion energy researchers. Typical fusion plasma experiments require real-time feedback for rapid tuning of experimental parameters, meaning data must be analyzed during the 15-minute intervals between plasma-generating pulses in experimental reactors. Such rapid assimilation of data is achieved by a geographically dispersed research team, a challenge for which LN technologies are well suited.

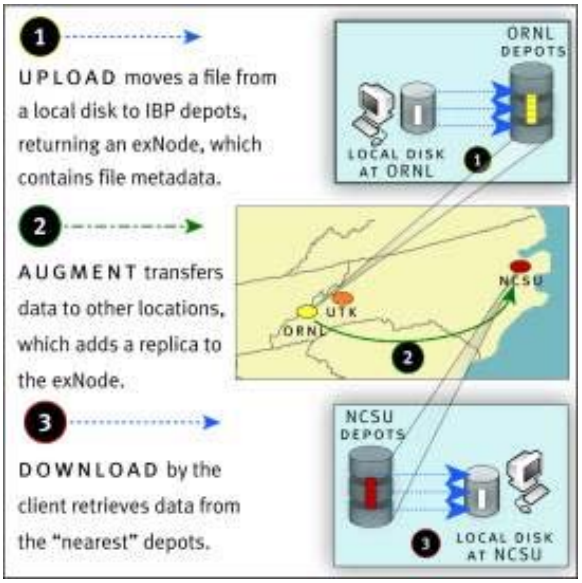


FIGURE 5: The interworking components of the Logistical Runtime System Tools (LoRS Tools) in the high performance distribution of data between IBP depots at Terascale Supernova Initiative sites at ORNL and NCSU.

Principal Investigator: Micah Beck, University of Tennessee

Estimating Bandwidth to Find the Fastest, Most Reliable Path

The **Bandwidth Estimation: Measurement Methodologies and Applications** project focused on the

research, development and deployment of scalable and accurate bandwidth estimation tools for high-capacity network links. Such tools would allow applications to adapt to changing network conditions, finding the fastest, most reliable network path. This adaptive ability would benefit a large class of data-intensive and distributed scientific applications. However, previous tools and methodologies for measuring network capacity, available bandwidth and throughput have been largely ineffective across real Internet infrastructures.

The goal was to develop measurement methodologies and tools for various bandwidth-related metrics, such as per-hop capacity, end-to-end capacity, and end-to-end available bandwidth. Capacity is the maximum throughput that the path can provide to an application when there is no competing traffic. Available bandwidth, on the other hand, is the maximum throughput that the path can provide to an application given the path's current traffic load. Measuring capacity is crucial for debugging, calibrating and managing a path, while measuring available bandwidth is important for predicting end-to-end performance of applications, for dynamic path selection and traffic engineering.

As part of the project, Georgia Tech researchers developed two bandwidth estimation tools, Pathrate (which measures capacity) and Pathload (which measures availability), which were released in January 2004. Pathrate and Pathload have been downloaded by more than 2,000 users around the world.

Principal Investigators: K. C. Klaffy, San Diego Supercomputer Center; Constantinos Davrolis, Georgia Institute of Technology

List of Publications

2001

K. Abazajian, G. M. Fuller, M. Patel, *"Sterile neutrino hot, warm, and cold dark matter,"* Physical Review D, **64**, 023501, 2001.

P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent and X.S. Li, *"Analysis and Comparison of Two General Sparse Solvers for Distributed Memory Computers,"* ACM Transactions on Mathematical Software, **27**:388-421, 2001.

S. F. Ashby, M. J. Holst, T. A. Manteuffel and P. E. Saylor, *"The Role of the Inner Product in Stopping Criteria for Conjugate Gradient Iterations,"* B.I.T., Vol **41**, No. 1, 2001.

N. R. Badnell, and D. C. Griffin, *"Electron-impact excitation of Fe^{20+}, including n=4 levels,"* Journal of Physics B, **34** 681, 2001.

N. R. Badnell, D. C. Griffin, and D. M. Mitnik, *"Electron-impact excitation of Fe21+, including n=4 levels,"* Journal of Physics B, **34**, 5071, 2001.

M. Baertschy and X. S. Li, *"Solution of a Three-Body Problem in Quantum Mechanics Using Sparse Linear Algebra on Parallel Computers,"* Proc. of the SC2001 conference, Denver, Colorado, November 2001.

M. Baker, *"Cluster Computing White Paper,"* International Journal of High Performance Computing Applications – special issue Cluster Computing White Paper, Vol. **15**, No. 2, Summer 2001.

S. Benson, L. Curfman McInnes, and J. More, *"A Case Study in the Performance and Scalability of Optimization Algorithms,"* ACM Transactions of Mathematical Software **27**:361-376, 2001.

J. M. Blondin, R. A. Chevalier, D. M. Frierson, *"Pulsar Wind Nebulae in Evolved Supernova Remnants,"* Astrophysical Journal Letters, **563**, 806-815, 2001.

J. M. Blondin, K. J. Borkowski, S. P. Reynolds, *"Dynamics of Fe Bubbles in Young Supernova Remnants,"* Astrophysical Journal Letters, **557**, 782-791, 2001.

M. Borland, H. Braun, S. Doebert, L. Groening, and A. Kabel, *"Recent Experiments on the Effect of Coherent Synchrotron Radiation on the Electron Beam of CTF II,"* Proc. of the 2001 Particle Accelerator Conference, Chicago, Ill., June 2001.

M. Brezina, A. Cleary, R. Falgout, V. Henson, J. Jones, T. Manteuffel, S. McCormick, and J. Ruge, 2001, *"Algebraic multigrid based on element interpolation (AMGe),"* SIAM Journal of Scientific Computing, **22**:1570-1592.

S. W. Bruenn, K. R. De Nisco, A. Mezzacappa, *"General Relativistic Effects in the Core Collapse Supernova Mechanism,"* Astrophysical Journal Letters, **560**, 326-338, 2001.

D. Bruhwiler, R. Giacone, J. Cary, J. Verboncoeur, P. Mardahl, E. Esarey, W. Leemans, B. Shadwick, *"Particle-in-Cell Simulations of Plasma Accelerators and Electron-Neutral Collisions,"* PRST-AB, **4**, 101302, 2001.

Z. Cai, T. Manteuffel, S. McCormick and J. Ruge, *"First-order System LL* (FOSLL*): Scalar Elliptic Partial Differential Equations,"* SIAM Journal on Numerical Analysis, **39**:1418-1445, 2001.

K. Campbell, *"Functional Sensitivity Analysis for Computer Model Output,"* Proc. of the Seventh Army Conference on Statistics, Santa Fe, NM, Oct. 2001.

H. Chen, et al., *"Calibrating Scalable Multi-Projector Displays Using Camera Homography Trees,"* Proc. of Computer Vision and Pattern Recognition, 2001.

H. Chen, et al., *"Data Distribution Strategies for High-Resolution Displays,"* Computers & Graphics, **25**(5):811-818, 2001.

T.-Y. Chen, *"Preconditioning sparse matrices for computing eigenvalues and computing linear systems of equations,"* PhD Dissertation, UC Berkeley. 2001.

Y. Chen, et al., *"Software Environments for Cluster-based Display Systems,"* Proc. of the First IEEE/ACM International Symposium on Cluster Computing and the Grid, 2001.

B. Cheng, J. Glimm, X. L. Li D. H. Sharp, *"Subgrid Models and DNS Studies of Fluid Mixing,"* Proceedings of the 7th International Conference on the Physics of Compressible Turbulent Mixing, E. Meshkov, Y. Yanilkin, V. Zhmailo, eds., p. 385-390, 2001.

E. Chow, *"Parallel Implementation and Practical Use of Sparse Approximate Inverses With A Priori Sparsity Patterns,"* International Journal of High Performance Computing Appl., **15**, pp. 56-74, 2001.

S. Chu, and S. Elliott, *"Latitude versus depth simulation of ecodynamics and dissolved gas chemistry relationships in the central Pacific,"* Journal of Atmospheric Chemistry, **40**(3), 305, 2001.

D. D. Clayton, E. A.-N. Deneault, B. S. Meyer, *"Condensation of Carbon in Radioactive Supernova Gas,"* Astrophysical Journal Letters, **562**, 480-493, 2001.

J. P. Colgan, M. S. Pindzola, D. M. Mitnik, D. C. Griffin, and I. Bray, *"Benchmark non-perturbative calculations for the electron-impact ionization of Li(2s) and Li(2p),"* Physical Review Letters, **87**, 213201, 2001.

J. P. Colgan, M. S. Pindzola, and F. J. Robicheaux, *"Fully quantal (Á, 2e) calcula-*

tions for absolute differential cross sections of helium," Journal of Physics B, **34**, L457, 2001.

V. K. Decyk and D. E. Dauger, *"Supercomputing for the Masses: A Parallel Macintosh Cluster,"* Proc. 4th Intl. Conf. on Parallel Processing and Applied Mathematics, Naleczow, Poland, September, 2001, Springer-Verlag Lecture Notes in Computer Science 2328, ed. by R. Wryrzykowski, J. Dongerra, M. Paprzycki, and J. Wasniewski Springer-Verlag, Berlin, 2002.

C. H. Q. Ding and Y. He, *"Ghost Cell Expansion Method for Reducing Communications in Solving PDE Problems,"* Proc of SC2001, Denver, Coloradao, Nov. 2001.

F. Dobrian, *"External Memory Algorithms for Factoring Sparse Matrices,"* PhD Dissertation, Old Dominion University, 2001.

F. Dobrian and A. Pothen, 2001, *"The Design of I/O-Efficient Sparse Direct Solvers,"* Proc. of the SC 2001 conference, Denver, Colorado, 2001.

V. Eijkhout, *"Automatic Determination of Matrix Blocks,"* Lapack Working note 151, Parallel Programming, 2001.

A. Gabric, W. Gregg, R. G. Najjar, D. J. Erickson III and P. Matrai, *"Modeling the biogeochemical cycle of DMS in the upper ocean: A review,"* Chemosphere - Global Change Science **3**, 377, 2001.

F. Gerigk, M. Vretenar, and R. D. Ryne, *"Design of the Superconducting Section of the SPL Linac at CERN,"* Proc. PAC 2001, p. 3909.

J. R. Gilbert, X. S. Li, E. G. Ng and B. W. Peyton, *"Computing Row and Column Counts for Sparse QR and LU Factorization,"* BIT **41**:693-710, 2001.

J. Glimm, X. L. Li, Y. J. Liu, N. Zhao, *"Conservative Front Tracking and Level Set Algorithms,"* Proc. National Academy of Sci., p. 14198-14201, 2001.

D. C. Griffin, D. M. Mitnik, J. P. Colgan and M. S. Pindzola, *"Electron-impact excitation of lithium,"* Physical Review A, **64**, 032718, 2001.

D. C. Griffin, D. M. Mitnik and N. R. Badnell, *"Electron-impact excitation of Ne^+,"* Journal of Physics B, **34**, 4401 2001.

E. D. Held, J. D. Callen, C. C. Hegna, and *C. R. Sovinec, "Conductive electron heat flow along magnetic field lines,"* Physics of Plasmas **8**, 1171, 2001.

P. Heggernes, S. Eisenstat, G. Kumfert and A. Pothen, *"The Computational Complexity of the Minimum Degree Algorithm,"* Proc. of the Nordic Computer Science Conference (NIK), 2001.

W. D. Henshaw, *"An Algorithm for Projecting Points onto a Patched CAD Model,"* Proc. of the 10th International Meshing Roundtable, October 2001.

I. Hofmann, O. Boine-Frankenheim, G. Franchetti, J. Qiang, R. Ryne, D. Jeon, J. Wei, *"Emittance Coupling in High Intensity Beams Applied to the SNS Linac,"* Proc. of the 2001 Particle Accelerator Conference, p. 2902, Chicago, Ill., June 2001.

I. Hofmann, J. Qiang, R. D. Ryne and R. W. Garnett, *"Collective Resonance Model of Energy Exchange in 3D Nonequipartitioned Beams,"* Physical Review Letters **86**, 2313–2316, 2001.

D. J. Holmgren, P. Mackenzie, D. Petravick, R. Rechenmacher and J. Simone, *"Lattice QCD production on a commodity cluster at Fermilab,"* Computing in High-Energy Physics and Nuclear, **2**, Beijing, China, Sept. 2001.

C. Huang, V. Decyk, S. Wang, E. S. Dodd, C. Ren, W. B. Mori, T. Katsouleas, and T. Antonsen Jr., *"QuickPIC: A Parallelized Quasi-Static PIC Code for Modeling Plasma Wakefield Acceleration,"* Proc. of the 2001 Particle Accelerator Conference, Chicago, Ill., June 2001.

E.-J. Im and K. A. Yelick, Paper: *"Optimizing Sparse Matrix-Vector Multiplication for Register Reuse,"* International Conference on Computational Science, San Francisco, Calif., May 2001

V. Ivanov, A. Krasnykh, *"Confined Flow Multiple Beam Guns for High Power RF Applications,"* Proc. of the 2nd IEEE International Vacuum Electronics Conference, Noordwijk, Netherlands, April 2001.

V. Ivanov, A. Krasnykh, *"3D Method for the Design of Multi or Sheet Beam RF Sources,"* Proc. of the 2001 Particle Accelerator Conference, Chicago, Ill., June 2001.

A. Kabel, *"Coherent Synchrotron Radiation Calculations Using TRAFIC4: Multi-processor Simulations and Optics Scans,"* Proc. of the 2001 Particle Accelerator Conference, Chicago, Ill., June 2001.

A. Kabel, *"Quantum Corrections to Intrabeam Scattering,"* Proc. of the 2001 Particle Accelerator Conference, Chicago, Ill., June 2001.

K. Keahey, T. Fredian, Q. Peng, D. P. Schissel, M. Thompson, I. Foster, M. Greenwald, and D. McCune, *"Computational Grids in Action,"* The National Fusion Collaboratory Future Generation Computer System, 2001.

S.-D. Kim, T. Manteuffel and S. McCormick, *"First-order system least squares (FOSLS) for spatial linear elasticity: pure traction,"* SIAM Journal on Numerical Analysis, **38**:1454-1482, 2001.

A. Kuprat, A. Khamayseh, *"Volume Conserving Smoothing for Piecewise Linear Curves, Surfaces, and Triple Lines,"* Journal of Computational Physics, **172**, p. 99-118, 2001.

C.-L. Lappen and D. A. Randall, *"Toward a Unified Parameterization of the Boundary Layer and Moist Convection. Part III: Simulations of Clear and Cloudy Convection,"* Journal of Atmospheric Sciences., **58**, 2052, 2001.

C.-L. Lappen and D. A. Randall *"Toward a Unified Parameterization of the Boundary Layer and Moist Convection. Part II: Lateral Mass Exchanges and Subplume-Scale Fluxes,"* Journal of Atmospheric Sciences., **58**, 2037, 2001.

C.-L. Lappen and D. A. Randall, *"Toward a Unified Parameterization of the Boundary Layer and Moist Convection. Part I: A New Type of Mass-Flux Model,"* Journal of Atmospheric Science, **58**, 2021, 2001.

J. Larson, R. Jacob, I. Foster, J. Guo, *"The Model Coupling Toolkit,"* Proc. of the. 2001 International Conference on Computational Science, eds. V. N. Alexandrov, J. J. Dongarra, C. J. K. Tan, Springer-Verlag, 2001.

S. Lee, T. Katsouleas, R. G. Hemker, E. S. Dodd, and W. B. Mori, *"Plasma-Wakefield Acceleration of a Positron Beam,"* Physical Review E, **64**, No. 4, 04550, 2001.

Z. Li, N. Folwell, G. Golub, A. Guetz, B. McCandless, C.-K. Ng, Y. Sun, M. Wolf, R. Yu and K. Ko, *"Parallel Computations of Wakefields in Linear Colliders and Storage Rings,"* Proc. of the 2001 Particle Accelerator Conference, Chicago, Ill., June 2001.

Z. Li, K. L. Bane, R. H. Miller, T. O. Raubenheimer, J. Wang, R. D. Ruth, *"Traveling Wave Structure Optimization for the NLC,"* Proc. of the 2001 Particle

Accelerator Conference, Chicago, Ill., June 2001.

Z. Li, P. Emma and T. Raubenheimer, *"The NLC L-band Bunch Compressor,"* Proc. of the 2001 Particle Accelerator Conference, Chicago, Ill., June 2001.

Z. Li, N. Folwell, G. Golub, A. Guetz, B. McCandless, C.-K. Ng, Y. Sun, M. Wolf, R. Yu and K. Ko, *"Parallel Computations Of Wakefields In Linear Colliders And Storage Rings,"* Proc. of the 2001 Particle Accelerator Conference, Chicago, Ill., June 2001.

Z. Liu, et al., *"Progressive View-Dependent Isosurface Propagation,"* Proc. of the IEEE TCVG Symposium on Visualization, 2001.

W. P. Lysenko et al., "*Characterizing Proton Beam of 6.7 MeV LEDA RFQ by Fitting Wire-Scanner Profiles to 3-D Nonlinear Simulations,"* Proc. of the 2001 Particle Accelerator Conference, p. 3051, Chicago, Ill., June 2001.

B. S. Meyer, S. S. Gupta, L.-S. The, S. Long, *"Long-Lived Nuclear Isomers and Short-Lived Radioactivities,"* Meteoritics & Planetary Science (Supp.) **36**, 134, 2001.

D. M. Mitnik, D. C. Griffin and N. R. Badnell, *"Electron-impact excitation of Ne^{5+},"* Journal of Physics B, **34**, 4455, 2001.

P. Muggli, et al., *"Collective refraction of a beam of electrons at a plasma-gas interface,"* Physical Review Letters Special Topics-Accelerators & Beams, Vol. **4**, No. 9, pp. 091301-091303, Sept. 2001.

S. Nath et al., *"Comparison of Linac Simulation Codes,"* Proc. of the 2001 Particle Accelerator Conference, p. 264, Chicago, Ill., June 2001.

J. Neiplocha, H. E. Trease, B. J. Palmer, D. R. Rector, *"Building an Application Domain Specific Programming Framework for Computational Fluid Dynamics Calculations on Parallel Computers,"* Tenth SIAM Conference on Parallel Processing for Scientific Computing, March 2001.

E. Parker, B. R. de Supinski and D. Quinlan, *"Measuring the Regularity of Array References,"* Los Alamos Computer Science Institute Symposium (LACSI 2001), Los Alamos, NM, Oct. 2001.

N. A. Peterson, K. K. Chand, *"Detecting translation errors in CAD surfaces and preparing geometries for mesh generation,"* Proc. of 10th Annual Meshing Round Table, Newport Beach, Calif., October 2001.

J. Pruet, K. Abazajian, G. M. Fuller, *"New connection between central engine weak physics and the dynamics of gamma-ray burst fireballs,"* Physical Review D, **64**, 063002, 2001.

J. Pruet, G. M. Fuller, C. Y. Cardall, *"On Steady State Neutrino-heated Ultrarelativistic Winds from Compact Objects,"* Astrophysical Journal Letters, **561**, 957-963, 2001.

S. C. Pryor, R. J. Barthelmie, J. T. Schoof, L. L. Sorensen, D. J. Erickson III, *"Implications of heterogeneous chemistry for nitrogen deposition to marine ecosystems: Observations and modeling,"* International Journal of Environmental Pollution, Water, Air and Soil Pollution, Focus **1**, 99, 2001.

J. Qiang and R. Ryne, *"Parallel 3D Poisson Solver for a Charged Beam in a Conducting Pipe,"* Computer Physics Communications **138**, 18, 2001.

J. Qiang, R. Ryne, B. Blind, J. Billen, T. Bhatia, R. Garnett, G. Neuschaefer, H. Takeda, *"High Resolution Parallel Particle-In-Cell Simulation of Beam Dynamics in the SNS Linac,"* Nuclear Instrument and Methods Physics, Res. A, **457**, 1, 2001.

J. Qiang, I. Hofmann, and R. D. Ryne, *"Cross-Plane Resonance: A Mechanism for Very Large Amplitude Halo Formation,"* Proc. of the 2001 Particle Accelerator Conference, p. 1735, Chicago, Ill., June 2001.

J. Qiang and R. D. Ryne, *"A Layer-Based Object-Oriented Parallel Framwork for Beam Dynamics Studies,"* Proc. of the 2001 Particle Accelerator Conference, p. 3060, Chicago, Ill., June 2001.

J. F. Remacle, M. S. Shephard, J. E. Flaherty, O. Klass, *"Parallel Algorithm oriented mesh database,"* Proc. 10th International Meshing Roundtable, p. 341-349, Newport Beach, Calif., October 2001.

R. Samanta, et al., *"Parallel Rendering with K-Way Replication,"* Proc. of the IEEE Symposium on Parallel and Large-Data Visualization and Graphics, 2001.

S. L. Scott, M. Brim, R. Flanery, A. Geist and B. Luethke, *"Cluster Command & Control (C3) Tools Suite,"* Parallel and Distributed Computing Practices – special issue, Nova Science Publishers, Inc., ISSN 1097-2803,Volume **4**, Number 4, Dec. 2001.

S. L. Scott, M. Brim and T. Mattson, *"OSCAR: Open Source Cluster Application Resources,"* 2001 Linux Symposium, Ottawa, Canada, July 2001.

S. L. Scott, M. Brim, G.A. Geist, B. Luethke and J. Schwidder, *"M3C: Managing and Monitoring Multiple Clusters,"* CCGrid 2001 – IEEE International Symposium on Cluster Computing and the Grid, Brisbane, Australia, May 2001.

M. Seth, K. G. Dyall, R. Shepard, and A. Wagner, *"The Calculation of f-f Spectra of Lanthanide and Actinide Ions by the MCDF-CI Method,"* Journal of Physics B: At. Molecular and Optical Physics **34**, 2383-2406 2001.

R. Shepard, A. F. Wagner, J. L. Tilson and M. Minkoff, *"The Subspace Projected Approximate Matrix (SPAM) Modification of the Davidson Method,"* Journal of Computational Physics **172**, 472-514. 2001.

A. Snavely, *"Modeling Application Performance by Convolving Machine Signatures with Application Profiles,"* IEEE 4th Annual Workshop on Workload Characterization, Austin, Texas, Dec. 2001.

C. R. Sovinec, J. M. Finn, and D. del-Castillo-Negrete, *"Formation and sustainment of spheromaks in the resistive MHD model,"* Physics of Plasmas **8**, 475, 2001.

L. Sugiyama, W. Park, H. R. Strauss, et al., *"Studies of spherical tori, stellarators, and anisotropic pressure with the M3D code,"* Nuclear Fusion **41**, 739, 2001.

K. Teranishi, P. Raghavan and E. G. Ng, *"Scalable Preconditioning Using Incomplete Factors,"* Proc. of the Tenth SIAM Conference on Parallel Processing for Scientific Computing, 2001.

T. A. Thompson, A. Burrows and B. S. Meyer, *"The Physics of Proto-Neutron Star Winds: Implications for r-Process Nucleosynthesis,"* Astrophysical Journal, **562**:887-908, Dec. 2001.

P. Vanek, M. Brezina and J. Mandel, *"Convergence analysis of algebraic multigrid based on smoothed aggregation,"* Numerical Mathematics **88**, 559–579, 2001.

R. Vuduc, J. Demmel and J. Bilmes, *"Statistical Models for Automatic Performance Tuning,"* International Journal of High Performance Computing Applications, 2001.

T. P. Wangler et al., *"Experimental Study of Proton-Beam Halo Induced by Beam Mismatch in LEDA,"* Proc. of the 2001 Particle Accelerator Conference, p. 2923, Chicago, Ill., June 2001.

A. D. Whiteford, N. R. Badnell, C. P. Ballance, M. G. O'Mullane, H. P. Summers and A. L. Thomas, *"A radiation-damped R-matrix approach to the electron-impact excitation of helium-like ions for diagnostic application to fusion and astrophysical plasmas,"* Journal of Physics B, **34**, 3179, 2001.

K. Wu, E. J. Otoo, and A. Shoshani, *"A performance comparison of bitmap indexes,"* Proc. of the 2001 ACM CIKM International Conference on Information and Knowledge Management, Atlanta, Georgia, USA, Nov. 2001.

2002

J. Abate, S. Benson, L. Grignon, P. Hovland, L. McInnes, and B. Norris, *"Integrating Automatic Differentiation with Object-Oriented Toolkits for High Performance Scientific Computing,"* From Simulation to Optimization, G. Corliss, C. Faure, A. Griewank, L. Hascoet and U. Naumann, eds, p 173-178, Springer-Verlag, New-York, 2002.

A. Adelmann, *"Space Charge Studies at PSI,"* Proc. 20th ICFA Advanced Beam Dynamics Workshop on High Brightness Hadron Beams (ICFA-HB 2002), p. 316, Batavia, Ill. April 2002.

A. Adelmann and D. Feichtinger, *"Generic Large Scale 3D Visualization of Accelerators and Beam Lines,"* Proc. ICCS 2002, p. 362, 2002.

S. Adjerid, K. D. Devine, J. E. Flaherty, L. Krivodonova, *"A posteriori error estimation for discontinuous Galerkin solutions of hyperbolic problems,"* Computer Methods in Applied Mechanics and Engineering, **191**, p. 1997-1112, 2002.

V. Akcelik, G. Biros and O. Ghattas, 2002, *"Parallel Multiscale Gauss-Newton-Krylov Methods for Inverse Wave Propagation,"* Proc. of the IEEE/ACM SC2002 Conference, Baltimore, Md., Nov. 2002.

W. Allcock, J. Bester, J. Bresnahan, I. Foster, J. Gawor, J. Insley, J. Link, M. Papka, *"GridMapper: A Tool for Visualizing the Behavior of Large-Scale Distributed Systems,"* Proc. of the 11th IEEE International Symposium on High Performance Distributed Computing HPDC-11, 179-188, 2002.

C. K. Allen, K. C. D. Chan, P. L. Colestock, K. R. Crandall, R. W. Garnett, J. D. Gilpatrick, W. Lysenko, J. Qiang, J. D. Schneider, M. E. Shulze, R. L. Sheffield, H. V. Smith, and T. P. Wangler, *"Beam-Halo Measurements in High-Current Proton Beams,"* Physical Review Letters, **89**, 214802, Nov. 2002.

J. Amundson and P. Spentzouris, *"A Hybrid, Parallel 3D Space Charge Code with Circular Machine Modeling Capabilities,"* Proc. of the International Computational Accelerator Physics Conference 2002 (ICAP2002), East Lansing, Michigan, Oct. 2002.

C. P. Ballance, N. R. Badnell, and K. A. Berrington, *"Electron-impact excitation of H-like Fe at high temperatures,"* Journal of Physics B, **35**, 1095, 2002.

G. P. Balls, P. Colella, *"A finite difference domain decomposition method using local corrections for the colution of Poissons's equation,"* Journal of Computational Physics, **180**, 25, 2002.

D. B. Batchelor, L. A. Berry, M. D. Carter, E. F. Jaeger, C. K. Phillips, R. Dumont, P. T. Bonoli, D. N. Smithe, R. W. Harvey, D. A. D'Ippolito, J. R. Myra, E. D'Azevedo, L. Gray and T. Kaplan, *"Tera-scale Computation of Wave-Plasma Interactions in Multidimensional Fusion Plasmas,"* Plasma Physics and Controlled Nuclear Fusion Research, 2002, Proc. of the 19th International Conference, Lyon, France, International Atomic Energy Agency, Vienna, 2002.

J. B. Bell, M. S. Day and J. F. Grcar, *"Numerical Simulation of Premixed Turbulent Methane Combustion,"* Proc. of the Combustion Institute, **29**:1987, 2002.

J. B. Bell, M. S. Day, J. F. Grcar, W. G. Bessler, C. Shultz, P. Glarborg and A. D. Jensen, *"Detailed Modeling and Laser-Induced Fluorescence Imaging of Nitric Oxide in an NH3-seeded non-premixed methane/air flame,"* Proc. of the Combustion Institute, 29:2195, 2002.

G. J. O. Beran, S. R. Gwaltney, and M. Head-Gordon, *"Can coupled cluster singles and doubles be approximated by a valence active space model?,"* Journal of Chemistry Physics. **117**, 3040-3048, 2002.

C. Bernard, et al. (The MILC Collaboration), *"Lattice Calculation of Heavy-Light Decay Constants with Two Flavors of Dynamical Quarks,"* Physical Review D **66**, 094501, 2002.

L. A. Berry, E. F. D'Azevedo, E. F. Jaeger, D. B. Batchelor and M. D. Carter, *"All-Orders, Full-Wave RF Computations Using Localized Basis Functions,"* 29th EPS Conference on Plasma Phys. and Contr. Fusion, ECA Vol. **26B**, P-4.109, June 2002.

G. Biros and O. Ghattas, *"Inexactness Issues in Lagrange-Newton-Krylov-Schur Methods for PDE-Constrained Optimization,"* Lecture Notes in Computational Science and Engineering, **30**, Springer-Verlag, 2002.

D. L. Brown, L. Freitag, J. Gilman, *"Creating interoperable meshing and discretization software: the Terascale Simulation Tools and Technology Center,"* Proc.of the Eighth International Conference on Numerical Grid Generation in Computational Field Simulations, Honolulu, Hawaii , June 2002.

X.-C. Cai and D. E. Keyes, *"Nonlinearly Preconditioned Inexact Newton Algorithms,"* SIAM Journal of Scientific Computing, **24**:183-200, 2002.

X.-C. Cai, D. E. Keyes and L. Marcinkowski, *"Nonlinear Additive Schwarz Preconditioners and Applications in Computational Fluid Dynamics,"* International Journal of Numerical Methods in Fluids, **40**:1463-1470, 2002.

X.-C. Cai, D. E. Keyes and D. P. Young, *"A Nonlinearly Additive Schwarz Preconditioned Inexact Newton Method for Shocked Duct Flow,"* Proc. of the 13th International Conference on Domain Decomposition Methods," (N. Debit et al., eds.) CIMNE pp. 345-352, 2002.

M. D. Carter, F. W. Baity, Jr., G. C. Barber, R. H. Goulding, Y. Mori, D. O. Sparks, K. F. White, E. F. Jaeger, F. R. Chang-Diaz, and J. P. Squire, *"Comparing*

Experiments with Modeling for Light Ion Helicon Plasma Sources," Physics of Plasmas **9**, 5097, 2002.

L. Chatterjee, M. R. Strayer, J. S. Wu, *"Pair production by neutrino bremsstrahlung,"* Physical Review D, **65**, 057302, 2002.

H. Chen, et al., *"Scalable Alignment of Large-Format Multi-Projector Displays Using Camera Homography Trees,"* Proc. of IEEE Visualization (VIZ), October 2002.

H. Chen, et al., *"Memory Performance Optimizations for Real-Time Software HDTV Decoding,"* Proc. of the IEEE International Conference on Multimedia and Expo, August 2002.

H. Chen, et al., *"A Parallel Ultra-High Resolution MPEG-2 Video Decoder for PC Cluster Based Tiled Display System,"* Proc. of International Parallel and Distributed Processing Symposium, 2002.

H. Chen, et al., *"Experiences with Scalability of Display Walls,"* Proc. of the 7th Annual Immersive Projection Technology Symposium, 2002.

E. Chow, T. A. Manteuffel, C. Tong, B. K. Wallin, "*Algebraic elimination of slide surface constraints in implicit structural analysis,"* International Journal for Numerical Methods in Eng., **01**, 1-21, 2002.

S. Chu, S. Elliott and M. Maltrud, *"Whole ocean fine resolution carbon management simulations systems,"* EOS, Transactions, American Geophysical Union 2002 Spring Meeting, **83**(19), S125, 2002.

C. E. Clayton, B. E. Blue, E. S. Dodd, C. Joshi, K. A. Marsh, W. B. Mori, S. Wang, P. Catravas, S. Chattopadhyay, E. Esarey, W. P. Leemans, R. Assmann, F. J. Decker, M. J. Hogan, R. Iverson, P. Raimondi, R. H. Siemann, D. Walz, T. Katsouleas, S. Lee and P. Muggli, *"Transverse Envelope Dynamics of a 28.5-GeV Electron Beam in a Long Plasma,"* Phys. Rev. Lett., **88**, 15 p. 154801/1-4, April 2002.

D. D. Clayton, B. S. Meyer, L.-S. The, M. F. El Eid, *"Iron Implantation in Presolar Supernova Grains,"* Astrophysical Journal Letters, **578**, L83-L86, 2002.

E. Colby, V. Ivanov, Z. Li, C. Limborg, *"Simulation Issues for RF Photoinjector,"* Proc. of the International Computational Accelerator Physics Conference 2002 (ICAP2002), East Lansing, Michigan, Oct. 2002.

J. P. Colgan and M. S. Pindzola, *"(Á, 2e) total and differential cross section calculations for helium at various excess energies,"* Physical Review A, **65**, 032729, 2002.

J. P. Colgan and M. S. Pindzola, *"Core-excited resonance enhancement in the two-photon complete fragmentation of helium,"* Physical Review Letters, **88**, 173002, 2002.

J. P. Colgan and M. S. Pindzola, *"Double photoionization of beryllium,"* Physical Review A, **65**, 022709, 2002.

J. P. Colgan and M. S. Pindzola, *"Time-dependent close-coupling studies of the electron-impact ionization of excited-state Helium,"* Physical Review A, **66**, 062707, 2002.

J. P. Colgan, M. S. Pindzola and F. J. Robicheaux, *"A Fourier transform method of calculating total cross sections using the time-dependent close-coupling theory,"* Physical Review A, **66**, 012718, 2002.

J. H. Cooley, T. M. Antonsen Jr., C. Huang, V. Decyk, S. Wang, E. S. Dodd, C. Ren, W. B. Mori, and T. Katsouleas, *"Further Developments for a Particle-in-Cell Code for Efficiently Modeling Wakefield Acceleration Schemes,"* Advanced Accelerator Concepts, Tenth Workshop, eds. C. E. Clayton and P. Muggli, AIP Conf. Proc. No. **647**, p. 232-239, 2002.

J. J. Cowan, C. Sneden, S. Burles, I. I. Ivans, T. C. Beers, J. W. Truran, J. E. Lawler, F. Primas, G. M. Fuller, B. Pfeiffer, K.-L. Kratz, *"The Chemical Composition and Age of the Metal-poor Halo Star BD +17°3248,"* Astrophysical Journal Letters, 572, 861-879, 2002.

T. Cristian, I.-H. Chung and J. K. Hollingsworth, *"Active Harmony: Towards Automated Performance Tuning,"* Proc. of the SC 2002 conference, Baltimore, Md., Nov. 2002.

S. Deng, F. Tsung, S. Lee, W. Lu, W. B. Mori, T. Katsouleas, P. Muggli, B. E. Blue., C. E. Clayton, C. O'Connell, E. Dodd, F. J. Decker, C. Huang, M. J. Hogan, R. Hemker, R. H. Iverson, C. Joshi, C. Ren, P. Raimondi, S. Wang and D. Walz, *"Modeling of Ionization Physics with the PIC Code OSIRIS,"* Advanced Accelerator Concepts, Tenth Workshop, eds. C. E. Clayton and P. Muggli, AIP Conf. Proc. No. **647**, p. 219-223, 2002.

S. Deng, T. Katsouleas, S. Lee, P. Muggli, W. B. Mori, R. Hemker, C. Ren, C. Huang, E. Dodd, B. E. Blue., C. E. Clayton, C. Joshi, S. Wang, F-J. Decker, M. J. Hogan, R. H. Iverson, C. O'Connell, P. Raimondi, and D. Walz, *"3-D Simulation of Plasma Wakefield Acceleration with Non-Idealized Plasmas and Beams,"* Advanced Accelerator Concepts, Tenth Workshop, eds. C. E. Clayton and P. Muggli, AIP Conf. Proc. No. **647**, p. 592-599. 2002.

L. Derose, K. Ekanadham, J. K. Hollingsworth and S. Sbaraglia, *"SIGMA: A Simulator to Guide Memory Analysis,"* Proc. of the SC 2002 conference, Baltimore, Md., Nov. 2002.

D. A. Dimitrov, D. L. Bruhwiler, W. Leemans, E. Esarey, P. Catravas, C. Toth, B. Shadwick, J. R. Cary, and R. Giacone, *"Simulations of Laser Propagation and Ionization in l'OASIS Experiments,"* Proc. Advanced, Accel. Concepts Workshop, p. 192, Mandalay Beach, CA, 2002.

D. A. Dimitrov, D. L. Bruhwiler, W. P. Leemans, E. Esarey, P. Catravas, C. Toth, B. A. Shadwick, J. R. Cary and R. E. Giacone, *"Simulations of Laser Propagation and Ionization in l'OASIS Experiments,"* Proc. Advanced Accel. Concepts Workshop, AIP Conf. Proc. 647, eds. C. E. Clayton and P. Muggli, AIP, New York, 2002.

E. S. Dodd, R. G. Hemker, C.-K.Huang, S. Wang, C. Ren, W. B. Mori, S. Lee and T. Katsouleas, *"Hosing and Sloshing of Short-Pulse Ge-V-Class Wakefield Drivers,"* Physical Review Letters, **88**, 125001, March 2002.

E. D. Dolan and J. J. More, *"Benchmarking Optimization Software with Performance Profiles,"* Mathematical Programming, **91**:201-213, 2002.

D. Dolgov, et al. (The LHPC Collaboration):, *"Moments of nucleon light cone quark distributions calculated in full lattice QCD,"* Physical Review D **66**, 034506, 2002.

S. C. Doney and M. W. Hecht, *"Antarctic Bottom Water Formation and Deep Water Chlorofluorocarbon Distributions in a Global Ocean Climate Model,"* Journal of Physics, Oceanography **32**, 1642, 2002.

R. J. Dumont, C. K. Phillips and D. N. Smithe, *"ICRF wave propagation and absorption in plasmas with non-thermal populations,"* 29th EPS Conference on Plasma Phys. and Contr. Fusion, ECA Vol. **26B**, P-5.051, Montreux, Switzerland, June 2002.

D. J. Erickson, III and J. L. Hernandez, *"A global, high resolution, satellite-based model of air-sea isoprene flux,"* Gas Transfer at Water Surfaces, ed. by M. A. Donelan, W. M. Drennan, E. S. Saltzman, and R. Wanninkhof, American Geophysical Union Monograph **127**, 312, p. 312, 2002.

R. Evard, D. Narayan, J. P. Navarro, and D. Nurmi, *"Clusters as large-scale development facilities,"* Proc of the 4th IEEE International Conference on Cluster Computing (CLUSTER02), p. 54, IEEE Computer Society, 2002.

R. D. Falgout and U. M. Yang, *"hypre: a Library of High Performance Preconditioners,"* in Computational Science - ICCS 2002 Part III, P. M. A. Sloot, C .J. K. Tan. J. J. Dongarra, and A. G. Hoekstra, eds., Lecture Notes in Computer Science, **2331**, p. 632-641, Springer-Verlag, 2002.

J. E. Flaherty, L. Krivodonova, J. F. Remacle, M. S. Shephard, *"Aspects of discontinuous Galerkin methods for hyperbolic conservation laws,"* Finite Elements in Analysis and Design, **38**:889-908, 2002.

J. E. Flaherty, L. Krivodonova, J. F. Remacle, M. S. Shephard, *"High-order adaptive and parallel discontinuous Galerkin methods for hyperbolic systems,"* WCCM V: Fifth World Congress on Computational Mechanics, Vienna Univ. of Tech., Vienna, Austria, p. 1:144, 2002.

R. A. Fonseca, et al., *"OSIRIS: A 3D, fully relativistic PIC code for modeling plasma based accelerators,"* Lect. Notes Comput. Sci, **2331**, 3 p. 342-351. 2002.

T. W. Fredian and J. A. Stillerman, *"MDSplus, Current Developments and Future Directions,"* The 3rd IAEA Technical Meeting on Control, Data Acquisition, and Remote Participation for Fusion Research, Fusion Engineering and Design, **60**, 229-233, 2002.

L. Freitag, T. Leurent, P. Knupp, D. Melander, *"MESQUITE Design: Issues in the Development of a Mesh Quality Improvement Toolkit",* Proceedings of the 8th Intl. Conference on Numerical Grid Generation in Computational Field Simulations, Honolulu, p159-168, 2002.

C. L. Fryer and M. S. Warren, *"Modeling Core-Collapse Supernovae in Three Dimensions,"* Astrophysical Journal Letters, **574**:L65-L68, July 2002.

G. Fubiani, G. Dugan, W. Leemans, E. Esarey, P. Catravas, C. Toth, B. Shadwick, J. R. Cary, and R. Giacone, *"Semi-analytical 6D Space Charge Model for Dense Electron Bunches with Large Energy Spreads,"* Proc. of the Advanced Accelerator Concepts Workshop Mandalay Beach, Calif., 2002.

G. M. Fuller, *"The nuclear physics and astrophysics of the new neutrino physics,"* AIP Conf. Proc. 610: Nuclear Physics in the 21st Century, p. 231-246, 2002.

A. Gebremedhin, F. Manne, and A. Pothen, *"Parallel Distance- k Coloring Algorithms for Numerical Optimization,"* Lecture Notes in Computer Science, **2400**, p. 912-921, Springer-Verlag, 2002.

E. George, J. Glimm, X. L. Li, A. Marchese, Z. L. Xu, *"A Comparison of Experimental, Theoretical and Numerical Simulation Rayleigh-Taylor Mixing Rates,"* Proc. National Academy of Science, **59**, p. 2587-2592, 2002.

S. J. Ghan, X. Bian, A. G. Hunt and A. Coleman, *"The thermodynamic influence of subgrid orography in a global climate model,"* Climate Dynamics, **20**, 31-44, 2002.

A. Z. Ghalam, T. Katsouleas, S. Lee, W. B. Mori, C. Huang, V. Decyk and C. Ren, *"Simulation of Electron-Cloud Instability in Circular Accelerators using Plasma Models,"* Advanced Accelerator Concepts, Tenth Workshop, eds. C. E. Clayton and P. Muggli, AIP Conf. Proc. No. **647**, p. 224j-231, 2002.

O. Ghattas and L. T. Biegler, *"Parallel Algorithms for Large-Scale Simulation-based Optimization,"* iModeling and Simulation-Based Life Cycle Engineering, Spon Press, London, 2002.

T. A. Gianakon, S. E. Kruger, and C. C. Hegna, *"Heuristic closures for numerical simulation of neoclassical tearing modes,"* Physics of Plasmas **9**, 536, 2002.

J. Glimm, X. L. Li, A. Lin, *"Nonuniform approach to terminal velocity for single mode Rayleigh-Taylor instability,"* Acta Mathematicae Applicatae Sinica, **18**, p. 1-8, 2002.

J. Glimm, X. L. Li, Y. J. Liu, *"Conservative Front Tracking in One Dimension,"* Fluid Flow and Transport in Porous Media: Mathematical and Numerical Treatment, Contemporary Mathematics, Z. X. Chen, R. Ewing, eds., American Mathematical Society, **295**, p. 253-264, 2002.

L. Griogori and X. S. Li, *"A New Scheduling Algorithm for Parallel Sparse LU Factorization with Static Pivoting,"* Proc. of the IEEE/ACM SC2002 Conference, Baltimore, Md., Nov. 2002.

W. Gropp, L. McInnes and B. Smith, *"Chapter 19 of CRPC Handbook of Parallel Computing,"* Morgan Kaufmann, 2002.

P. T. Haertel and D. A. Randall, *"Could a pile of slippery sacks behave like an ocean?"* Monthly Weather Review, **130**, 2975, 2002.

A. Heger, S. E.Woosley, T. Rauscher, R. D. Horman, and M. M. Boyes, *"Massive star evolution: nucleosynthesis and nuclear reaction rate uncertainties,"* New Astronomy Review, **46**:463-468, July 2002.

R. P. Heikes, *"A comparison of vertical coordinate systems for numerical modeling of the general circulation of the atmosphere,"* Ph.D. thesis, Colorado State University, 2002.

W. D. Henshaw, *"Generating Composite Overlapping Grids on CAD Geometries,"* Numerical Grid Generation in Computational Field Simulations, June 2002.

W. D. Henshaw, *"An Algorithm for Projecting Points onto a Patched CAD Model,"* Engineering with Computers, **18**, p. 265-273, 2002.

V. E. Henson and U. M. Yang, *"BoomerAMG: a Parallel Algebraic Multigrid Solver and Preconditioner,"* Applied Numerical Mathematics, **41**, p. 155-177, 2002.

J. J. Heys, C. G. DeGroff, T. Manteuffel, S. McCormick and W. W. Orlando, *"First-order system least squares for elastohydrodynamics with application to flow in compliant blood vessels,"* Biomed. Sci. Instrum. **38**, p. 277-282, 2002.

M. J. Hogan, C. D. Barnes, C. E. Clayton, C. O'Connell, F. J. Decker, S. Deng, P. Emma, C. Huang, R. Iverson, D. K. Johnson, C. Joshi, T. Katsouleas, P. Krejcik, W. Lu, K. A. Marsh, W. B. Mori, P. Muggli, R. H. Siemann and D. Walz, *"Acceleration and Focusing of Electrons and Positrons using a 30 GeV Drive Beam,"* Advanced Accelerator Concepts, Tenth Workshop, eds. C. E. Clayton and P. Muggli, AIP Conf. Proc. No. **647**, pp. 3-10, 2002.

P. Hovland, B. Norris and B. Smith, *"Making Automatic Differentiation truly Automatic: Coupling PETSc with ADIC,"* Proc. of ICCS 2002, Amsterdam, Netherlands, 2002.

E. C. Hunke and J. K. Dukowicz, *"The Elastic-Viscous-Plastic Sea Ice Dynamics Model in General Orthogonal Curvilinear Coordinates on a Sphere–Incorporation of Metric Terms,"* Monthly Weather Review, **130**, 1848, 2002.

C. Joshi, B. Blue, C. E. Clayton, E. Dodd, C. Huang, K. A. Marsh, W. B. Mori, S. Wang, J. J. Hogan, C. O'Connell, R. Siemann, D. Watz, P. Muggli, T. Katsouleas and S. Lee, *"High Energy Density Plasma Science with an Ultrarelativistic Electron Beam,"* Physics of Plasmas, Vol. **9**, No. 5, p. 1845-1855, May 2002.

J. Ivanic and K. Ruedenberg, "*Deadwood in Configuration Spaces. II. SD and SDTQ Spaces,"* Theoretical Chemistry Accounts, **107**, 220-228, 2002.

V. Ivanov, N. Folwell, G. Golub, A. Guetz, Z. Li, W. Mi, C.-K. Ng, G. Schussman, Y. Sun, J. Tran, M. Weiner, M. Wolf and K. Ko, *"Computational Challenge In Large Scale Accelerator Modeling,"* ICCM-2002, Novosibirsk, Russia, June 2002.

V. Ivanov, R. Ives, A. Krasnykh, G. Miram, M. Read, *"An Electron Gun for a Sheet Beam Klystron,"* IVEC-2002, Monterey, Calif., April 2002.

V. Ivanov, G. Schussman, M. Weiner, *"Particle Tracking Algorithms for 3D Parallel Codes in Frequency and Time Domains,"* Proc. of 18th Annual Review of Progress in Applied Computational Electromagnetics, ACES-2002, Monterey, Calif., March 2002.

E. F. Jaeger, L. A. Berry, E. D'Azevedo, D. B. Batchelor, M. D. Carter, K. F. White and H. Weitzner, *"Advances in Full-Wave Modeling of Radio Frequency Heated, Multidimensional Plasmas,"* Physics of Plasmas **9**, 1873, 2002.

G. C. Jordan, B. S. Meyer, *"Sensitivity of Isotope Yields to Reaction Rates in the Alpha Rich Freezeout,"* Proc. of the Workshop on Astrophysics, Symmetries, and Applied Physics at Spallation Neutron Sources (ASAP 2002), p. 42. Oak Ridge, Tenn. March 2002.

A. Kabel, "*A Parallel Code for Lifetime Calculations in P/P-Storage Rings in the Presence of Parasitic Beam-Beam Crossings,"* Proc. of the International Computational Accelerator Physics Conference 2002 (ICAP2002), East Lansing, Michigan, Oct. 2002.

A. Kabel, *"Parallel Simulation Algorithms for the Strong-Strong Beam-Beam Interaction,"* Proc. of the International Computational Accelerator Physics Conference 2002 (ICAP2002), East Lansing, Michigan, Oct. 2002.

T. Katsouleas, A. Z. Ghalam, S. Lee, W. B. Mori, C. Huang, V. Decyk and C. Ren, *"Plasma Modeling of Wakefields in Electron Clouds,"* ECLOUD'02 Mini-Workshop on Electron-Cloud Simulations for Proton and Positron Beams, CERN, Geneva, Switzerland, 2002.

K. Keahey and V. Welch, *"Fine-Grain Authorization for Resource Management in the Grid Environment,"* Proc. of the 3rd International Workshop on Grid Computing, 2002.

D. E. Keyes, *"Terascale Implicit Methods for Partial Differential Equations,"* The Barrett Lectures, University of Tennessee Mathematics Department, 2001, Contemporary Mathematics **306**:29-84, AMS, Providence, RI, 2002.

D. E. Keyes, P. D. Hovland, L. C. McInnes and W. Samyono, *"Using Automatic Differentiation for Second-Order Matrix-free Methods in PDE-constrained Optimization,"* Automatic Differentiation of Algorithms: From Simulation to Optimization (G. Corliss et al., eds.), Springer-Verlag, p 35-50, 2002.

A. Khamayseh, A. Kuprat, *"Hybrid Curve Point Distribution Algorithms,"* SIAM Journal on Scientific Computing, **23**, p. 1464-1484, 2002.

A. Klawonn, O. B. Widlund and M. Dryja, *"Dual-Primal FETI Methods for Three-dimensional Elliptic Problems with Heterogeneous Coefficients,"* SIAM Journal on Numerical Analysis, **40**:159-179, 2002.

K. Ko, *"High Performance Computing in Accelerator Physics,"* Proc. of 18th Annual Review of Progress in Applied Computational Electromagnetics, ACES-2002, Monterey, Calif., March 2002.

S. Lee, T. Katsouleas, P. Muggli, W. B. Mori, C. Joshi, R. Hemker, E. S. Dodd, C. E. Clayton, K. A. Marsh, B. Blue, S. Wang, R. Assmann, F. J. Decker, M. Hogan, R. Iverson, and D. Walz, *"Energy Doubler for a Linear Collider,"* Physical Review Special Topics-Accelerators And Beams, **5**, 1, January 2002.

X. Li, J. Demmel, D. Bailey, G. Henry, Y. Hida, J. Iskandar, W. Kahan, S. Kang, A. Kapur, M. Martin, B. Thompson, T. Tung and D. Yoo, *"Design, Implementation and Testing of Extended and Mixed Precision BLAS,"* ACM Transactions of Mathematical Software **22**:152-205, 2002.

M. Liebendorfer, O. E. B. Messer, A. Mezzacappa, W. R. Hix, F.-K. Thielemann, K. Langanke, *"The importance of neutrino opacities for the accretion luminosity in spherically symmetric supernova models,"* Proc. of the 11th Workshop on Nuclear Astrophysics, p. 126-131, Max-Planck-Institut fuer Astrophysik, Germany, 2002.

Z. Liu, et al., *"Improving Progressive View-Dependent Isosurface Propagation,"* Computers and Graphics, **26** (2): 209-218, 2002.

S. D. Loch, M. S. Pindzola and J. P. Colgan, *"Electron-impact ionization of all ionization stages of krypton,"* Physical Review A, **66**, 052708, 2002.

C.-D. Lu and D. A. Reed, *"Compact Application Signatures for Parallel and Distributed Scientific Codes,"* Proc. of the SC 2002 conference, Baltimore, Md., Nov. 2002.

X. Luo, M. S. Shephard, J. F. Remacle, R. M. Bara, M. W. Beall, B. A. Szab, *"p-Version Mesh Generation Issues,"* 11th International Meshing Roundtable, 2002.

X. Luo, M. S. Shephard, J. F. Remacle, *"The Influence of Geometric Approximation on the Accuracy of High Order Methods,"* Proc. 8th International Conference on Numerical Grid Generation in Computational Field Simulations, Miss. State University, 2002.

W. P. Lysenko, R. W. Garnett, J. D. Gilpatrick, J. Qiang, L. J. Rybarcyk, R. D. Ryne, J. D. Schneider, H. V. Smith, L. M. Young, and M. E. Schulze, *"High Order Beam Features and Fitting Quadrupole Scan Data to Particle Code Model,"* Proc. of the International Computational Accelerator Physics Conference 2002 (ICAP2002), East Lansing, Michigan, Oct. 2002.

K.-L. Ma, G. Schussman, B. Wilson, K. Ko, J. Qiang and R. Ryne, *"Advanced Visualization Technology for Terascale Particle Accelerator Simulations,"* Proc. of the IEEE/ACM SC2002 Conference, Baltimore, Md., Nov. 2002.

J. L. McClean, P.-M. Poulain, J. W. Pelton, and M. E. Maltrud, *"Eulerian and Lagrangian statistics from surface drifters*

and a high-resolution POP simulation in the North Atlantic," Journal of Physical Oceanography, **32**, 2472, 2002.

C. W. McCurdy, P. Cummings, E. Stechel, B. Hendrickson and D. E. Keyes, *"Theory and Modeling in Nanoscience,"* whitepaper commissioned by the U.S. DOE Offices of Basic Energy Sciences and Advanced Scientific Computing, 2002.

C. L. Mendes and D. A. Reed, *"Monitoring Large Systems via Statistical Sampling,"* LACSI Symposium, Santa Fe, Oct. 2002.

B. S. Meyer, *"r-Process Nucleosynthesis without Excess Neutrons,"* Physical Review Letters, **89**, 231101, 2002.

D. M. Mitnik, D. C. Griffin, and M. S. Pindzola, *"Time-dependent close-coupling calculations of dielectronic capture in He,"* Physical Review Letters, **88**, 173004, 2002.

J. J. More, *"Automatic Differentiation Tools in Optimization Software,"* in Automatic Differentiation 2000: From Simulation to Optimization, G. Corliss, C. Faure, A. Griewank, L. Hascoet, and U. Naumann, eds, p 25-34, Springer-Verlag, New-York, 2002.

W. B. Mori, *"Recent Advances and Some Results in Plasma-Based Accelerator Modeling,"* Advanced Accelerator Concepts, Tenth Workshop, eds. C. E. Clayton and P. Muggli, AIP Conf. Proc. No. **647**, p. 11-28, 2002.

P. Muggli, *"Transverse Envelope Dynamics of a 28.5-GeV Electron Beam in a Long Plasma,"* Physical Review Letters, Vol. **88**, No. 15 pp. 154801/1-4, April 2002.

C. Naleway, M. Seth, R. Shepard, A. F. Wagner, J. L. Tilson, W. C. Ermler and S. R. Brozell, *"An Ab Initio Study of the Ionization Potentials and the f-f Spectroscopy of Europium Atoms and Ions,"* Journal of Chemistry Physics. **116**, 5481-5493. 2002.

J. P. Navarro, R. Evard, D. Nurmi, and N. Desai, *"Scalable cluster administration - {Chiba City I} approach and lessons learned,"* Proc of the 4th IEEE International Conference on Cluster Computing (CLUSTER02), p. 54, IEEE Computer Society, 2002.

J.W. Negele, *"Understanding parton distributions from lattice QCD: Present limitations and future promise,"* Nuclear Physics A **711**, 281, 2002.

C.-K. Ng, L. Ge, A. Guetz, V. Ivanov, Z. Li, G. Schussmann, Y. Sun, M. Weiner, M. Wolf, *"Numerical Studies of Field Gradient and Dark Currents in SLAC Structures,"* Proc. of the International Computational Accelerator Physics Conference 2002 (ICAP2002), East Lansing, Michigan, Oct. 2002.

C.-K. Ng et. al., *"Modeling HOM Heating in the PEP-II IR with Omega3P,"* Proc. of the International Computational Accelerator Physics Conference 2002 (ICAP2002), East Lansing, Michigan, Oct. 2002.

B. Norris, S. Balay, S. Benson, L. Freitag, P. Hovland, L. McInnes, and B. Smith, *"Parallel Components for PDEs and Optimization: Some Issues and Experiences,"* Parallel Computing **28**:1811-1831, 2002.

C. O'Connell et al., *"Dynamic Focusing of an Electron Beam through a Long Plasma,"* Phys. Rev. STAB, **5**, 121301, 2002.

R. J. Oglesby, S. Marshall, D. J. Erickson III, J. O. Roads and F. R. Robertson, *"Thresholds in atmosphere-soil moisture interactions: Results from climate model studies,"* Journal of Geophysical Research,. **107**, 2002.

L. F. Pavarino and O. B. Widlund, *"Balancing Neumann-Neumann methods for incompressible Stokes equations,"* Comm. Pure Appl. Math. **55**:302-335, 2002.

M. S. Pindzola, *"Proton-impact excitation of laser-excited lithium atoms,"* Physical Review A, **66**, 032716, 2002.

P. Ploumans, G. S. Winckelmans, J. K. Salmon, A. Leonard, and M. S. Warren, *"Vortex Methods for High-Resolution Simulation of Three-Dimensional Blu® Body Flows; Application to the Sphere at Re=300, 500 and 1000,"* Journal of Computational Physics, **178**:427-463, 2002.

J. Pruet and N. Dalal, *"Implications of Neutron Decoupling in Short Gamma-Ray Bursts,"* ApJ, **573**:770-777, July 2002.

J. Pruet, S. Guiles, G. M. Fuller, *"Light-Element Synthesis in High-Entropy Relativistic Flows Associated with Gamma-Ray Bursts,"* Astrophysical Journal Letters, **580**, 368-373, 2002.

J. Qiang, P. L. Colestock, D. Gilpatrick, H. V. Smith, T. P. Wangler and M. E. Schulze, *"Macroparticle Simulation Studies of a Proton Beam Halo Experiment,"* Phys. Rev. ST Accel. Beams, vol **5**, 124201, 2002.

J. Qiang, M. Furman and R. Ryne, *"Strong-Strong Beam-Beam Simulation Using a Green Function Approach,"* Phys. Rev. ST Accel. Beams, **5**, 104402, Oct. 2002.

J. Qiang and R. Ryne, *"Parallel Beam Dynamics Simulation of Linear Accelerators,"* Proceedings of the 2002 Applied Computational Electromagnetics Society (ACES'2002) Conference, March 2002.

D. A. Randall, T. D. Ringler, R. P. Heikes, P. Jones and J. Baumgardner, *"Climate modeling with spherical geodesic grids,"* Computing in Science and Engr., **4**, 32-41. 2002.

T. Rauscher, A. Heger, R. D. Hoffman and S. E. Woosley, *"Nucleosynthesis in Massive Stars with Improved Nuclear and Stellar Physics,"* American Physics Journal, **576**:323-348, Sept. 2002.

J. F. Remacle, O. Klass, J. E. Flaherty, M. S. Shephard, *"A parallel algorithm oriented mesh database,"* Engineering with Computers, **18**, 274,2002.

J. F. Remacle, M. S. Shepard, J. E. Flaherty, *"Some issues on distributed mesh representations,"* Proc. 8th International Conference on Numerical Grid Generation in Computational Field Simulations, Miss. State University, 2002.

J. F. Remacle, O. Klass, M. S. Shephard, *"Trellis: A framework for adaptive numerical analysis based on multiparadigm programming in C++,"* WCCM V: Fifth World Congress on Computational Mechanics, Vienna Univ. of Tech, Vienna, Austria, p. 1-164, 2002.

J. F. Remacle, X. Li, N. Chevaugeon, M. S. Shepard, *"Transient mesh adaptation using conforming and non-conforming mesh modifications,"* 11th International Meshing Roundtable, 2002.

T. D. Ringler and D. A. Randall, *"The ZM Grid: An Alternative to the Z Grid,"* Monthly Weather Review, **130**, 1411–1422, 2002.

T. D. Ringler, and D. A. Randall, *"A Potential Enstrophy and Energy Conserving Numerical Scheme for Solution of the Shallow-Water Equations on a Geodesic Grid,"* Monthly Weather Review, **130**, 1397–1410, 2002.

F. J. Robicheaux and J. D. Hanson, *"Simulation of the expansion of an ultracold neutral plasma,"* Physical Review Letters, **88**, 055002. 2002.

J. M. Sampaio, K. Langanke, G. Martinez-Pinedo, D. J. Dean, *"Neutral-current neutrino reactions in the supernova environment,"* Physics Letters B, **529**, 19-25. 2002.

D. P. Schissel, M. J. Greenwald, and W .E. Johnston, *"Fusion Energy Sciences Networking: A Discussion of Future Requirements,"* DOE High Performance Network Planning Workshop, 2002.

D. P. Schissel, *"An Advanced Collaborative Environment to Enhance Magnetic Fusion Research, for the National Fusion Collaboratory Project,"* Proceedings of the Workshop on Advanced Collaborative Environments, 2002.

D. P. Schissel, et al., *"Data Management, Code Deployment, and Scientific Visualization to Enhance Scientific Discovery in Fusion Research through Advanced Computing,"* The 3rd IAEA Technical Meeting on Control, Data Acquisition, and Remote Participation for Fusion Research. Fusion Engineering and Design **60**, 481-486, 2002.

K. L. Schuchardt, J. D. Myers, E. G. Stephan, 2002, *"A web-based data architecture for problem-solving environments: application of distributed authoring and versioning the extensible computational chemistry environment,"* Cluster Computing **5**(3):287-296, 2002.

D. R. Schultz, C. O. Reinhold, P. S. Krstic and M. R. Strayer, *"Ejected-electron spectrum in low-energy proton-hydrogen collisions,"* Physical Review A, **65**, 052722, 2002.

G. Schussman and K.-L. Ma, *"Scalable Self-Orienting Surfaces: A Compact, Texture-Enhanced Representation for Interactive Visualization Of 3D Vector Fields,"* Proc. of the Pacific Graphics 2002 Conference, Beijing, China, Oct. 2002.

G. Schussman and K.-L. Ma, *"Scalable Self-Orienting Surfaces: A Compact Texture-Enhanced Representation for Interactive Visualization Of 3d Vector Fields,"* Proc. of the 10th Pacific Conference on Computer Graphics and Applications, IEEE Computer Society, Washington, D.C., Oct. 2002.

S. L. Scott, B. Luethke and T. Naughton, *"C3 Power Tools – The Next Generation,"* 4th DAPSYS Conference, Linz, Austria, Sept.–Oct. 2002.

S. L. Scott, B. Luethke, *"HPC Federated Cluster Administration with C3 v3.0,"* Ottawa Linux Symposium (OLS 2002), Ottawa, Canada, July 2002.

S. L. Scott, J. L. Mugler and T. Naughton, *"User Interfaces for Clustering Tools,"* Ottawa Linux Symposium (OLS 2002), Ottawa, Canada, July 2002.

S. L. Scott, B. Luethke, *"C3 Power Tools Commodity, High-Performance Cluster Computing Technologies and Applications,"* Sixth World Multiconference on Systemics, Cybernetics, and Informatics (ISAS SCI2002), Orlando, Fla., July 2002.

S. L. Scott, T. Naughton, B. Barrett, J. Squyres, A. Lumsdain and Y. C. Fang, *"The Penguin in the Pail – OSCAR Cluster Installation Tool Commodity, High-Performance Cluster Computing Technologies and Applications,"* Sixth World Multiconference on Systemics, Cybernetics, and Informatics (ISAS SCI2002), Orlando, Fla., July 2002.

B. A. Shadwick, G. M. Tarkenton, E. H. Esarey and W. P. Leemans, *"Fluid simulations of intense laser-plasma interactions,"* IEEE Trans. Plasma Sci. **30**, 38, 2002.

M. S. Shephard, X. Luo, J. F. Remacle, *"Meshing for p-version finite element methods,"* WCCM V: Fifth World Congress on Computational Mechanics, Vienna Univ. of Tech, Vienna, Austria, p. 1-464, 2002.

A. Snavely, et al., *"A Framework for Application Performance Modeling and Prediction,"* Proc. of the SC 2002 conference, Baltimore, Md., Nov. 2002.

P. Spentzouris, J. Amundson, J. Lackey, L. Spentzouris, R. Tomlin, *"Space Charge Studies and Comparison with Simulations Using the FNAL Booster,"* Proc. of the International Computational Accelerator Physics Conference 2002 (ICAP2002), East Lansing, Michigan, Oct. 2002.

N. Sullivan, A. D. Jensen, P. Glarborg, M. S. Day, J. F. Grcar, J. B. Bell, C. J. Pope, and R. J. Kee, *"Ammonia Conversion and NOx Formation in Laminar Coflowing Nonpremixed Methane-Air Flames,"* Combustion and Flame, **131**(3):285, 2002.

Y. Sun, N. Folwell, Z. Li and G. H. Golub, *"High Precision Accelerator Cavity Design Using the Parallel Eigensolver Omega3p,"* Proc. of 18th Annual Review of Progress in Applied Computational Electromagnetics, ACES-2002, Monterey, Calif., March 2002.

Y. Sun, G. Golub and K. Ko, *"Solving the Complex Symmetric Eigenproblem in Accelerator Structure Design,"* Proc. of the International Computational Accelerator Physics Conference 2002 (ICAP2002), East Lansing, Michigan, Oct. 2002.

K. Teranishi, P. Raghavan, and E. G. Ng, *"A New Data-Mapping Scheme for Latency-Tolerant Distributed Sparse Triangular Solution,"* Proc. of the IEEE/ACM SC2002 Conference, Baltimore, Md., Nov. 2002.

K. Teranishi, P. Raghavan, and E. G. Ng, *"Reducing Communication Costs for Parallel Sparse Triangular Solution,"* Proc. of the IEEE/ACM SC2002 Conference, Baltimore, Md., Nov. 2002.

F.-K. Thielemann, D. Argast, F. Brachwitz, G. Martinez-Pinedo, T. Rauscher, M. Liebendoerfer, A. Mezzacappa, P. Hoflich, K. Nomoto, *"Nucleosynthesis and Stellar Evolution,"* Astrophysics and Space Science, **281**, 25-37, 2002.

F.-K Thielemann,. D. Argast, F. Brachwitz, G. Martinez-Pinedo, T. Rauscher, M. Liebendoerfer, A. Mezzacappa, P. Hoflich, K. Iwamoto, K. Nomoto, *"Nucleosynthesis in Supernovae. (I),"* ASP Conf. Ser. 253: Chemical Enrichment of Intracluster and Intergalactic Medium, p. 205, 2002.

F.-K. Thielemann, P. Hauser, E. Kolbe, G. Martinez-Pinedo, I. Panov, T. Rauscher, K.-L. Kratz, B. Pfeiffer, S. Rosswog, M. Liebendoerfer, A. Mezzacappa, *"Heavy Elements and Age Determinations,"* Space Science Reviews, **100**, 277-296, 2002.

J. L. Tilson, C. Naleway, M. Seth, R. Shepard, A. F. Wagner, and W. C. Ermler, *"An Ab Initio Study of the f-f Spectroscopy of Americium+3,"* Journal of Chemistry Physics. **116**, 5494-5502, 2002.

S. J. Thomas, J. M. Dennis, H. M. Tufo, P. F. Fischer, *"A Schwarz preconditioner for the cubed-sphere,"* Proc. of the Copper Mountain Conference on Iterative Methods, 2002.

H. Trease, L. Trease, J. Fowler, R. Corley, C. Timchalk, K. Minard, D. Rommeriem, *"A Case Study: Extraction, Image Reconstruction, And Mesh Generation From NMR Volume Image Data From F344 Rats For Computational Biology Applications,"* 8th International Conference on Grid Generation and Computational Physics, 2002.

F. S. Tsung., R. G. Hemker, C. Ren, W. B. Mori, L. O. Silva and T. Katsouleas,

"Generation of Ultra-Intense, Single-Cycle Laser Pulse using Photon Deceleration," Proceedings of the National Academy of Sciences., Vol. **99**, pp. 29-32, 2002.

T. Van Voorhis and M. Head-Gordon, *"Implementation of generalized valence-bond inspired coupled cluster theories,"* Journal of Chemical Physics, **117**, 9190-9201, 2002.

J. L. Vay, P. Colella, P.McCorquodale, B. Van Straalen, A. Friedman, D.P. Grote, *"Mesh refinement for particle-in-cell plasma simulations: Applications to and benefits for heavy ion fusion,"* Laser and Particle Beams, **20**, 4, p. 569-575, 2002.

J. S. Vetter and P. Worley, *"Asserting Performance Expectations,"* Proc. of the SC 2002 conference, Baltimore, Md., Nov. 2002.

J. S. Vetter and A. Yoo, *"An Empirical Performance Evaluation of Scalable Scientific Applications,"* Proc. of the SC 2002 conference, Baltimore, Md., Nov. 2002.

J. S. Vetter, *"Dynamic Statistical Profiling of Communication Activity in Distributed Applications,"* Proc. of SIGMETRICS 2002: Joint International Conference on Measurement and Modeling of Computer Systems, ACM, 2002.

J. S. Vetter and F. Mueller, *"Communication Characteristics of Large-Scale Scientific Applications for Contemporary Cluster Architectures,"* Proc. of the International Parallel and Distributed Processing Symposium, 2002.

R. Vuduc, J. W. Demmel, K. A. Yelick, S. Kamil, R. Nishtala and B. Lee, *"Performance Optimizations and Bounds for Sparse Matrix-Vector Multiply,"* Proc. of the IEEE/ACM SC2002 Conference, Baltimore, Md., Nov. 2002.

R. Vuduc, S. Kamil, J. Hsu, R. Nishtala, J. W. Demmel and K. A. Yelick, *"Automatic Performance Tuning and Analysis of Sparse Triangular Solve,"* ICS 2002: Workshop on Performance Optimization via High-Level Languages and Libraries, 2002.

G. Wallace, *"Display Wall Cluster Management,"* Proc. of the IEEE Visualization 2002 Workshop on Commodity-Based Visualization Clusters, Oct. 2002.

S. Wang, C. E. Clayton, B. E. Blue, E. S. Dodd, K. A. Marsh, W. B. Mori, C. Joshi, P. Muggli, T. Katsouleas, F. J. Decker, M. J. Hogan, R. H. Iverson, P. Raimondi, D. Watz, R. Siemann, and R. Assmann, *"X-ray Emission from Betatron Motion in a Plasma Wiggler,"* Physical Review Letters, Vol. **88**, No. 13, p. 135004/1-4, April 2002.

A. Wetzels, A. Gurtler, L. D. Noordam, F. Robicheaux, C. Dinu, H. G. Muller, M. J. J. Vrakking and W. J. van der Zande, *"Rydberg state ionization by half-cycle-pulse excitation: strong kicks create slow electrons,"* Physical Review Letters, **89**, 273003. 2002.

A. D. Whiteford, N. R. Badnell, C. P. Ballance, S. D. Loch, M. G. O'Mullane and H. P. Summers, *"Excitation of Ar15+ and Fe23+ for diagnostic application to fusion and astrophysical plasmas,"* Journal of Physics B, **35**, 3729, 2002.

B. Wilson, K.-L. Ma and P. McCormick, *"A Hardware-Assisted Hybrid Rendering Technique for Interactive Volume Visualization,"* 2002 Symposium on Volume Visualization and Graphics, Boston, Mass., Oct. 2002.

B. Wilson, K.-L. Ma, J. Qiang, and R. Ryne, *"Interactive Visualization of Particle Beams for Accelerator Design,"* In Proceedings of the Workshop on Particle Accelerator Science and Technology, ICCS 2002, Amsterdam, Netherlands, April 2002.

M. Wingate, et al. (The HPQCD Collaboration), *"Heavy Light Physics Using NRQCD/Staggered Actions,"* Nuclear Physics B (Proc. Suppl.) **106**, 379, 2002.

M. Wolf, A. Guetz and C.-K. Ng, *"Modeling Large Accelerator Structures with the Parallel Field Solver Tau3P,"* Proc. of 18th Annual Review of Progress in Applied Computational Electromagnetics, ACES-2002, Monterey, Calif., March 2002.

C. S. Woodward, K. E. Grant and R. Maxwell, *"Applications of Sensitivity Analysis to Uncertainty Quantification for Variably Saturated Flow,"* Computational Methods in Water Resources, S.M. Hassanizadeh, R. J. Schotting, W. G. Gray, and G. F. Pinder, eds., vol.**1**, pp. 73-80, Elsevier, Amsterdam, 2002.

S. E. Woosley, A. Heger, and T. A. Weaver, *"The evolution and explosion of massive stars,"* Reviews of Modern Physics, **74**:1015-1071, Nov. 2002.

P. H. Worley, *"Scaling the Unscalable: A Case Study on the AlphaServer SC,"* Proc. of the IEEE/ACM SC2002 Conference, Baltimore, Md., Nov. 2002.

P. H. Worley, T. H. Dunigan, Jr., M. R. Fahey, J. B. White III, A. S. Bland, *"Early Evaluation of the IBM p690,"* Proc. of the IEEE/ACM SC2002 Conference, Baltimore, Md., Nov. 2002.

K. Wu, J. Ekow, E. J. Otoo, and A. Shoshani, *"Compressing bitmap indexes for faster search operations,"* Proc. of SSDBM'02, p. 99, Edinburgh, Scotland, 2002.

M. Zingale, L. J. Dursi, J. ZuHone, A. C. Calder, B. Fryxell, T. Plewa, J. W. Truran, A. Caceres, K. Olson, P. M. Ricker, K. Riley, R. Rosner, A. Siegel, F. X. Timmes and N. Vladimirova, *"Mapping Initial Hydrostatic Models in Godunov Codes,"* Astrophysical Journal Supplement, **143**:539-565, Dec. 2002.

2003

S. I. Abarzhi, J. Glimm, A. D. Lin, *"Rayleigh-Taylor instability for fluids with a finite density contrast,"* Phys. Fluids, **15**, p. 2190-2197, 2003.

S. I. Abarzhi, J. Glimm, K. Nishihara, *"Rayleigh-Taylor instability and Richtmyer-Meshkov instabilities for fluids with a finite density contrast,"* Phys. Lett. A, **11**, p. 1-7, 2003.

M. Adams, M. Brezina, J. Hu, and R. Tuminaro, *"Parallel multigrid smoothing: polynomial versus Gauss-Seidel,"* Journal of Computational Physics, **188**, p. 593-610, 2003.

V. Akcelik, J. Bielak, G. Biros, I. Epanomeritakis, A. Fernandez, O. Ghattas, E. J. Kim, D. O'Hallaron and T. Tu, 2003, *"High-resolution Forward and Inverse Earthquake Modeling on Terascale Computers,"* Proc. of the ACM/IEEE SC03 conference, Nov. 2003.

C. Alexandrou et al., *"Calculation of the N to Delta electromagnetic transition matrix element,"* Nuclear Physics B (Proc. Suppl.) **119**, 413, 2003.

P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent and X. S. Li, *"Impact of the Implementation of MPI Point-to-Point Communications on the Performance of Two General Sparse Solvers,"* Parallel Computing, **29**:833-849, 2003.

J. Amundson, J. Lackey, P. Spentzouris, G. Jungman, L. Spentzouris, *"Calibration of the Fermilab Booster ionization profile monitor,"* Physics Review ST Accel. Beams. **6**, 102801, 2003.

J. Amundson, P. Spentzouris, *"FNAL Booster: Experiment and Modeling,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

J. Amundson, P. Spentzouris, *"SYNERGIA: A Hybrid, Parallel Beam Dynamics Code with 3D Space Charge,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

C. Aubin, et al. (The MILC Collaboration), *"Chiral logs with staggered fermions,"* Nuclear Physics B (Proc. Suppl.), **119**, 233, 2003.

N. R. Badnell, D. C. Griffin, and D. M. Mitnik, *"Electron-impact excitation of B+ using the R-matrix with pseudo-states method,"* Journal of Physics B, **1337** 2003.

N. R. Badnell, M. G. O'Mullane, H. P. Summers, Z. Altun, M. A. Bautista, J. P. Colgan, T. W. Gorczyca, D. M. Mitnik, M. S. Pindzola, and O. Zatsarinny, *"Dielectronic recombination data for dynamic finite-density plasmas: I. Goals and methodology,"* Astronomy and Astrophysics, **406**, 1151, 2003.

A. B. Balantekin, G. M. Fuller, *"Supernova neutrino nucleus astrophysics,"* Journal of Physics G, **29**, 2513-2522, 2003.

C. P. Ballance, N. R. Badnell and E. S. Symth, *"A pseudo-state sensitivity study on hydrogenic ions,"* Journal of Physics B, **36**. 3707. 2003.

C. P. Ballance, N. R. Badnell, D. C. Griffin, S. D. Loch and D. M. Mitnik, *"The effects of coupling to the target continuum on the electronimpact excitation of Li+,"* Journal of Physics B, **36**, 235, 2003.

G. T. Balls, S. B. Baden, P. Colella, *"SCALLOP: A highly scalable parallel Poisson solver in three dimensions,"* Proc. of ACM/IEEE SC03 conference, Phoenix, Arizona, November, 2003.

M. W. Beall, J. Walsh, M. S. Shephard, *"A comparison of techniques for geometry access related to mesh generation,"* Proc. 7th US Nat. Congress on Comp. Mech., p. 62, 2003.

M. W. Beall, J. Walsh, M. S. Shephard., *"Accessing CAD geometry for mesh generation,"* 12th International Meshing Roundtable, Sandia National Laboratories, p. 33-42, 2003.

J. B. Bell, M. S. Day, J. F. Grcar, M. J. Lijewski, M. Johnson, R. K. Cheng and I. G. Shepherd, *"Numerical Simulation of a Premixed Turbulent V-Flame,"* 19th International Colloquium on the Dynamics of Explosions and Reactive Systems, July-Aug. 2003.

J. B. Bell, M. S. Day, A. S. Almgren, R. K. Cheng, and I. G. Shepherd, *"Numerical Simulation of Premixed Turbulent Methane Combustion,"* Proc. of the Second MIT Conference on Computational Fluid and Solid Mechanics, June 2003.

J. B. Bell, M. S. Day, J. F. Grcar, and M. J. Lijewski, *"Analysis of carbon chemistry in numerical simulations of vortex flame interactions,"* 19th International Colloquium on the Dynamics of Explosions and Reactive Systems, July-Aug. 2003.

C. Bernard, et al. (The MILC Collaboration), *"Topological Susceptibility with the Improved Asqtad Action,"* Phys. Rev. D **68**, 114501, 2003.

C. Bernard, et al. (The MILC Collaboration), *"Light hadron properties with improved staggered quarks,"* Nuclear Physics B (Proc. Suppl.), **119**, 257, 2003.

C. Bernard, et al. (The MILC Collaboration), *"Topological susceptibility with the improved Asqtad action,"* Nuclear Physics B (Proc. Suppl.), **119**, 991, 2003.

C. Bernard, et al. (The MILC Collaboration), *"Static hybrid quarkonium potential with improved staggered quarks,"* Nuclear Physics B (Proc. Suppl.), **119**, 598, 2003.

C. Bernard, et al. (The MILC Collaboration), *"High temperature QCD with three flavors of improved staggered quarks,"* Nuclear Physics B (Proc. Suppl.), **119**, 523, 2003.

C. Bernard, et al. (The MILC Collaboration), *"Exotic hybrid mesons from improved Kogut-Susskind fermions,"* Nuclear Physics B (Proc. Suppl.), **119**, 260, 2003.

C. Bernard, et al. (The MILC Collaboration), *"Heavy–light meson decay constants with Nf =3,"* Nuclear Physics B (Proc. Suppl.), **119**, 613, 2003.

C. Bernard, et al. (The MILC Collaboration), *"Lattice calculation of 1?+ hybrid mesons with improved Kogut-Susskind fermions,"* Physical Review D **68**, 074505, 2003.

S. Bhowmick, L. McInnes, B. Norris, and P. Raghavan, 2003, *"The Role of Multi-Method Linear Solvers in PDE-based Simulations,"* Proc. of the 2003 International Conference on Computational Science and its Applications, Montreal, Canada, Lecture Notes in Computer Science, **2677**, p. 828-839, V. Kumar, M. L. Gavrilova, C. J. K. Tan, and P. L'Ecuyer. eds, May 2003.

L. Biegler, O. Ghattas, M. Heinkenschloss and B. van Bloemen Waanders, editors, *"PDE-Constrained Optimization: State-of-the-Art,"* Lecture Notes in Computational Science and Engineering, 30, Springer-Verlag, 2003.

J, M. Blondin, *"The Inherent Asymmetry of Core-Collapse Supernovae,"* ASP Conf. Ser. **293**: 3D Stellar Evolution, p. 290, 2003.

J. M. Blondin, A. Mezzacappa, C. DeMarino, *"Stability of Standing Accretion Shocks, with an Eye toward Core-Collapse Supernovae,"* Astrophysical Journal Letters, **584**, 971-980, 2003.

B. E. Blue et al., *"Plasma-Wakefield Acceleration of an Intense Positron Beam,"* Phys. Rev. Lett. **90**, 214801, 2003.

P. A. Boyle, C. Jung and T. Wettig, *"The QCDOC supercomputer: Hardware, software, and performance,"* Econf C0303241, THIT003, 2003.

M. Branstetter, and D. J. Erickson III, *"Continental runoff dynamics in the CCSM2.0,"* Journal of Geophysical Research **108**(D17), 4550, 2003.

D. P. Brennan, R. J. La Haye, A. D. Turnbull, et al., *"A mechanism for tearing onset near ideal stability boundaries,"* Physics of Plasmas **10** 1643, 2003.

J. A. Breslau, S. C. Jardin and W. Park, *"Simulation studies of the role of reconnection in the 'current hole' experiments in the joint European torus,"* Physics of Plasmas **10** 1665, 2003.

M. Brewer, L. Diachin, T. Leurent, D. Melander, *"The Mesquite Mesh Quality Improvement Toolkit,"* Proc. of the 12th International Meshing Roundtable, Santa Fe NM, p. 239-250, 2003.

P. N. Brown, B. Lee, T. A. Manteuffel, *"A moment-parity multigrid preconditioner for the first-order least-squares formulation of the Blotzmann transport equations,"* SIAM Journal of Scientific Computing, **25**, 2, p. 513-533, 2003.

P. N. Brown, P. Vassilevski, and C. S. Woodward, *"On Mesh-Independent Convergence of an Inexact Newton-Multigrid Algorithm,"* SIAM Journal of Scientific Computing, **25**, 2, p. 570-590, 2003.

D. L. Bruhwiler, D. A. Dimitrov, J. R. Cary, E. Esarey, W. P. Leemans and R. E. Giacone, *"Particle-in-cell simulations of tunneling ionization effects in plasma-based accelerators,"* Physics of Plasmas **10**, p. 2022, 2003.

D. L. Bruhwiler, D. A. Dimitrov, J. R. Cary, E. Esarey and W. P. Leemans, *"Simulation of ionization effects for high-density positron drivers in future plasma wakefield experiments,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

N. Bucciantini, J. M. Blondin, L. Del Zanna, E. Amato, *"Spherically symmetric relativistic MHD simulations of pulsar wind nebulae in supernova remnants,"* Astronomy & Astrophysics, **405**, 617-626, 2003.

T. Burch and D. Toussaint (The MILC Collaboration), *"Hybrid configuration content of heavy S-wave mesons,"* Physical Review D, **68**, 094504, 2003.

R. Butler, D. Narayan, A. Lusk and E. Lusk, *"The process management component of a scalable system software environment,"* Proc. of the 5th IEEE International Conference on Cluster Computing (CLUSTER03), Kowloon, Hong Kong, Dec. 2003.

L. Bytautas, J. Ivanic, K. Ruedenberg, *"Split-Localized Orbitals Can Yield Stronger Configuration Interaction Convergence than Natural Orbitals,"* Journal of Chemical Physics, **119**, 8217, 2003.

C. Cardall, A. Mezzacappa, *"Conservative formulations of general relativistic kinetic theory,"* Physical Review D, **68**, 023006, 2003.

L. Carrington, A. Snavely, N. Wolter, and X. Gao, *"A Performance Prediction Framework for Scientific Applications,"* ICCS Workshop on Performance Modeling and Analysis (PMA03), Melbourne, Australia, June 2003.

M. D. Carter, F. W. Baity Jr., G. C. Barber, R. H. Goulding, Y. Mori, D. O. Sparks, K. F. White, E. F. Jaeger, F. R. Chang-Diaz and J. P. Squire, *"Comparing Experiments with Modeling to Optimize Light Ion Helicon Plasma Sources for VASIMR,"* Proc. of Open Systems, Korea, Transactions of Fusion Science and Technology **43**(1), 2003.

J. R. Cary, R. E. Giacone, C. Nieter, D. L. Bruhwiler, E. Esarey, G. Fubiani and W. P. Leemans, *"All-Optical Beamlet Train Generation,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

G. K. L. Chan and M. Head-Gordon, *"Exact solution (in a triple zeta, double polarization basis) of the Schrödinger electronic equation for water,"* Journal of Chemical Physics, **118**, 8851-8854, 2003.

B. Cheng, J. Glimm, H. Jin, D. H. Sharp, *"Theoretical methods for the determination of mixing,"* Laser and Particle Beams, **21**, p. 429-436, 2003.

N. Chevaugeon, J. E. Flaherty, L. Krivodonova, J. F. Remacle, M. S. Shephard, *"Adaptive and parallel discontinuous Galerkin method for hyperbolic conservation law,"* Proc. 7th US Nat. Congress on Comp. Mech., p. 448, 2003.

N. Chevaugeon, J. F. Remacle, J. E. Flaherty, D. Cler, M. S. Shephard, *"Application of discontinuous Galerkin method. Large scale problem: Cannon blast modeling,"* Proc. 7th US Nat. Congress on Comp. Mech., p. 470, 2003.

Y. Choi, S. Elliott, D. R. Blake, F. S. Rowland, et al., *"PCA survey of whole air hydrocarbon data from the second airborne BIBLE expedition,"* Journal of Geophysical Research, **108**, 10, 2003.

T. Chartier, R. D. Falgout, V. E. Henson, J. Jones, T. Manteuffel, S. McCormick, J. Ruge and P. S. Vassilevski, *"Spectral AMGe (ÚAMGe),"* SIAM Journal of Scientific Computing, **25**, p. 1-26, 2003.

E. Chow, *"An Unstructured Multigrid Method Based on Geometric Smoothness,"* Numer. Linear Algebra Appl., **10**, p. 401-421, 2003.

E. Chow, T. A. Manteuffel, C. Tong and B. K. Wallin, *"Algebraic Elimination of Slide Surface Constraints in Implicit Structural Analysis,"* Intern. Journal on Numerical Analysis,. Meth. Engrg., **57**, p. 1129-1144, 2003.

E. Chow and P. Vassilevski, *"Multilevel Block Factorizations in Generalized Hierarachical Bases,"* Numer. Linear Algebra Appl., **10**, p. 105-127, 2003.

S. Chu, S. M. Elliott, and M. E. Maltrud, *"Global eddy permitting simulations of surface ocean nitrogen, iron, sulfur cycling,"* Chemosphere, **50**, 223, 2003.

S. Chu, S. Elliott, M. Maltrud, F. Chai and F. Chavez, *"Studies of the consequences of ocean carbon sequestration using Los Alamos ocean models,"* Proceedings of the DOE 2nd Annual Conference on Carbon Sequestration, Alexandria, Va., May 2003.

D. L. Cler, N. Chevaugeon, M. S. Shephard, J. E. Flaherty, J. F. Remacle, *"CFD application to gun muzzle blast - A validation case study,"* 41st AIAA Aerospace Sciences Meeting and Exhibit, Jan. 2003.

A. Codd, T. Manteuffel and S. McCormick, *"Multilevel first-order system least squares for nonlinear elliptic partial differential equations,"* SIAM Journal on Numerical Analysis, **41**, p. 2197-2209, 2003.

A. Codd, T. Manteuffel, S, McCormick and J. Ruge, *"Multilevel first-order system least squares for elliptic grid generation,"* SIAM Journal on Numerical Analysis, **41**, pp. 2210-2232, 2003.

J. P. Colgan, M. S. Pindzola, A. D. Whiteford, and N. R. Badnell, *"Dielectronic recombination data for dynamic finite-density plasmas: III. The Beryllium isoelectronic sequence,"* Astronomy and Astrophysics, **412**, 597, 2003.

J. P. Colgan and M. S. Pindzola, *"Total and differential cross section calculations for the double photoionization of the helium 1x2s1,3 S states,"* Physical Review A, **67**, 012711, 2003.

J. P. Colgan, M. S. Pindzola, and F. J. Robicheaux, *"Time-dependent studies of single and multiple photoionization of H2+,"* Physical Review A, **68**, 063413, 2003.

J. P. Colgan, M. S. Pindzola, and M. C. Witthoeft, *"Time-dependent electron-impact scattering from He+ using variable lattice spacings,"* Physical Review A, 032713, 2003.

J. P. Colgan, S. D. Loch, M. S. Pindzola, C. P. Ballance, and D. C. Griffin, *"Electron-impact ionization of all ionization stages of Beryllium,"* Physical Review A, 032712, 2003.

D. Datta, C. Picu, M. S. Shephard, *"Multiscale simulation of defects using multigrid atomistic continuum method,"* Proc. 7th US Nat. Congress on Comp. Mech., p. 814, 2003.

C. Davies, et al. (The HPQCD Collaboration), *"The Determination of Alpha(s) from Lattice QCD with 2+1 Flavors of Dynamical Quarks,"* Nuclear Physics B (Proc. Suppl.), **119**, 595, 2003.

J. Demmel and Y. Hida, *"Accurate Floating Point Summation,"* SIAM Journal of Scientific Computing, **25**, 4, p. 1214–1248, 2003.

S. Dey, L. Couchman, D. Datta, *"Error and convergence of p-refinement schemes for elastodynamics and coupled elasto-acoustics,"* Proc. 7th US Nat. Congress on Comp. Mech., , p. 517, 2003.

M. di Pierro et al., *"Charmonium with three flavors of dynamical quarks,"* Nuclear Physics B (Proc. Suppl.) **119**, 586, 2003.

J. Dongarra, K. London, S. Moore, P. Mucci, D. Terpstra, H. You, and M. Zhou, *"Experiences and Lessons Learned with a Portable Interface to Hardware Performance Counters,"* PADTAD Workshop, IPDPS 2003, Nice, France, April 2003.

J. Dongarra and V. Eijkhout, *"Self-adapting Numerical Software and Automatic Tuning of Heuristics,"* ICCS 2003, Workshop on Adaptive Algorithms, Melbourne, Australia, June 2003.

J. Dongarra, A. Malony, S. Moore, P. Mucci, and S. Shende, *"Performance Instrumentation and Measurement for Terascale Systems,"* ICCS 2003, Terascale Systems Workshop, Melbourne, Australia, June 2003.

P. Dreher, et al. (The SESAM Collaboration), *"Continuum extrapolation of moments of nucleon quark distributions in full QCD,"* Nuclear Physics B (Proc. Suppl.), **119**, 392, 2003.

M. Dryja and O. Widlund, *"A Generalized FETI-DP Method for a Mortar Discretization of Elliptic Problems,"* Proc of the 14th International Symposium on Domain Decomposition Methods, Cocoyoc, Mexico, Jan. 2002, I. Herrera, D. E. Keyes, O. B. Widlund and R. Yates eds., 2003.

R. J. Dumont, C. K. Phillips, A. Pletzer and D.N. Smithe, "*Effects of Non-Maxwellian Plasma Species on ICRF Wave Propagation and Absorption in Toroidal Magnetic Confinement Devices,"* invited paper in the 10th European Fusion Theory Conference, Helsinki, Finland, Sept. 2003.

R. J. Dumont, C. K. Phillips, and D. N. Smithe, *"Effects of Non-Maxwellian Plasma Species on ICRF Propagation and Absorption,"* Radio Frequency Power in Plasmas, Proc. 15th Topical Conf., Moran, Wyoming, 2003, AIP, N. Y., 2003.

T. H. Dunigan, Jr., M. R. Fahey, J. B. White III, P. H. Worley, *"Early Evaluation of the Cray X1,"* Proc. of the ACM/IEEE SC03 conference, Phoenix, Ariz., Nov. 2003.

L. J. Dursi, M. Zingale, A. C. Calder, B. Fryxell, F. X. Timmes, N. Vladimirova, R. Rosner, A. Caceres, D. Q. Lamb, K. Olson, P. M. Ricker, K. Riley, A. Siegel, and J. W. Truran, *"The Response of Model and Astrophysical Thermonuclear Flames to Curvature and Stretch,"* ApJ, **595**:955-979, Oct. 2003.

S. Dutta, E. George, J. Glimm, X. L. Li, A. Marchese, Z. L. Xu, Y. M. Zhang, J. W. Grove, D. H. Sharp, *"Numerical methods for the determination of mixing,"* Laser and Particle Beams, **21**, p. 437-442, 2003.

S. Dutta, J. Glimm, J. W. Grove, D. H. Sharp, Y. Zhang, "*A fast algorithm for moving interface problems,"* International Conference on Computational Science and Its Applications (ICCSA 2003), Lecture Notes in Computer Science 2668, V. Kumar et al.., ed., Springer-Verlag, Berlin/Heidelberg, p. 782-790, 2003.

S. Elliott and S. Chu, *"Comment on 'ocean fertilization experiments initiate large scale phytoplankton blooms,'"* Geophysical Research Letters, **30**, 1274, 2003.

S. Elliott, and H. Hanson, *"Syndication of the Earth system,"* Environmental Science and Policy, **6**, 457, 2003.

S. Elliott, D. R. Blake, F. S. Rowland, et al., *"Whole air sampling as a window on Pacific biogeochemistry,"* Journal of Geophysical Research, **108**(D3), 8407, 2003.

D. J. Erickson III, J. Hernandez, P. Ginoux, W. Gregg, C. McClain, and J. Christian, *"Atmospheric Iron Delivery and surface ocean biological activity in the Southern Ocean and Patagonian region,"* Geophysical Research Letter, **30**(12), 1609, 2003.

J. Fetter, G. C. McLaughlin, A. B. Balantekin, G. M. Fuller, *"Active-sterile neutrino conversion: consequences for the r-process and supernova neutrino detection,"* Astroparticle Physics, **18**, 433-448, 2003.

P. Fischer, F. Hecht, Y. Maday, *"A Parareal in Time Semi-implicit Approximation of the Navier-Stokes Equations,"* Proc. Of the 15th Int. Conf. on Domain Decomposition Methods, Berlin, 2003.

P. F. Fischer, J. W. Lottes, *"Hybrid Schwarz-Multigrid Methods for the Spectral Element Method: Extensions to Navier-Stokes,"* Proc. Of the 15th Int. Conf. on Domain Decomposition Methods, Berlin, 2003.

N. Folwell, P. Knupp *"Increasing Tau3P Abort-Time via Mesh Quality Improvement,"* Proceedings of the 12th International Meshing Roundtable, Santa Fe NM, p. 379-392, 2003.

N. Folwell, P. Knupp and M. Brewer, *"Increasing the TAU3P Abort-time via Mesh Quality Improvement,"* Proc. of the 12th International Meshing Roundtable, Sandia National Laboratories, Santa Fe, NM, Sept. 2003.

N. Folwell, P. Knupp, K. Ko, *"Mesh Quality Improvement for Accelerator Design,"* SIAM Conference on Computational Science and Engineering, San Diego, Calif., Feb. 2003.

C. L. Fryer and P. Meszaros, *"Neutrino-driven Explosions in Gamma-Ray Bursts and Hypernovae,"* ApJ Letters, **588**:L25-L28, May 2003.

G. Fubiani, E. Esarey, W. Leemans, J. Qiang, R. D. Ryne and G. Dugan, *"Numerical Studies of Laser-Plasma Produced Electron Beam Transport,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

G. M. Fuller, A. Kusenko, I. Mocioiu, S. Pascoli, *"Pulsar kicks from a dark-matter sterile neutrino,"* Physical Review D, **68**, 103002, 2003.

E. Gabriel, G. Fagg and J. Dongarra, *"Evaluating the Performance of MPI-2 Dynamic Communicators and One-sided Communication,"* EuroPVM/MPI 2003, Venice, Italy, Sept. 2003.

Z. Gan, Y. Alexeev, R. A. Kendall, and M. S. Gordon, *"The Parallel Implementation of a Full CI Program,"* Journal of Chemical Physics, **119**, 47, 2003.

X. Gao and A. Snavely, *"Exploiting Stability to Reduce Time-Space Cost for Memory Tracing,"* ICCS Workshop on Performance Modeling and Analysis (PMA03), Melbourne, Australia, June 2003.

E. George, J. Glimm, J. W. Grove, X. L. Li, Y. J. Liu, Z. L. Xu, N. Zhao, *"Simplification, conservation and adaptivity in the front tracking method,"* in Hyperbolic Problems: Theory, Numerics, Applications, T. Hou, E. Tadmor, eds., Springer Verlag, Berlin and New York, p. 175-184200, 2003.

F. X. Giraldo, J. B. Perot and P. F. Fischer, *"A spectral element semi-Lagrangian (SESL) method for the spherical shallow water equations,"* J. of Comp. Phys., **190** 2, p. 623-650, 2003.

J. Glimm, S. Hou, Y. Lee, D. Sharp, K. Ye, *"Solution error models for uncertainty quantification,"* Contemporary Mathematics, **327**, p. 115-140, 2003.

J. Glimm, H. Jin, M. Laforest, F. Tangerman, Y. Zhang, *"A two pressure numerical model of two fluid mixing,"* SIAM J. Multiscale Model. Simul., **1**, p. 458-484, 2003.

J. Glimm, Y. Lee, D. H. Sharp, K. Q. Ye, *"Prediction using numerical simulations, A Bayesian framework for uncertainty quantification and its statistical challenge,"* in Proceedings of the Fourth International Symposium on Uncertainty Modeling and Analysis (ISUMA 2003), B. M. Ayyub, N. O. Attoh-Okine, eds., IEEE Computer Society, 2003.

J. Glimm, X. L. Li, Y. J. Liu, Z. L. Xu, N. Zhao, *"Conservative front tracking with improved accuracy,"* SIAM J. Numerical Analysis, **41**, p. 1926-1947, 2003.

J. Glimm, X. L. Li, W. Oh, A. Marchese, M.-N. Kim, R. Samulyak, C. Tzanos, *"Jet breakup and spray formation in a diesel engine,"* Proc. of the Second MIT Conference on Computational Fluid and Solid Mechanics, Cambridge, Mass., 2003.

P. Goldfeld, 2003, *"Balancing Neumann-Neumann for (In)Compressible Linear Elasticity and (Generalized) Stokes - Parallel Implementation,"* Proc of the 14th International Symposium on Domain Decomposition Methods, Cocoyoc, Mexico, Jan. 2002, I. Herrera, D. E. Keyes, O. B. Widlund and R. Yates, eds., 2003.

P. Goldfeld, L. F. Pavarino and O. B. Widlund, *"Balancing Neumann-Neumann Preconditioners for Mixed Approximations of Heterogenous Problems in Linear Elasticity,"* Numer. Math., **95**, 283-324, 2003.

D. A. Goussis, M. Valorani, F. Creta, and H. N. Najm, *"Inertial Manifolds with CSP,"* Computational Fluid and Solid Mechanics, **1**:1951-1955, K. J. Bathe, ed., Elsevier, 2003.

A. Gray, et al. (The HPQCD Collaboration), *"The Upsilon Spectrum from Lattice QCD with 2+1 Flavors of Dynamical Quarks,"* Nuclear Physics B (Proc. Suppl.), **119**, 592, 2003.

J. F. Grcar, M. S. Day and J. B. Bell, *"Conditional and opposed reaction path diagrams for the analysis of fluid-chemistry interactions,"* 19th International Colloquium on the Dynamics of Explosions and Reactive Systems, July-Aug. 2003.

D. C. Griffin, J. P. Colgan, S. D. Loch, M. S. Pindzola, and C. P. Ballance *"Electron-impact excitation of beryllium and its ions,"* Physical Review A, **68**, 062705, 2003.

A. T. Hagler, et al. (The LHPC Collaboration), *"Moments of nucleon generalized parton distributions in lattice QCD,"* Physical Review D **68**, 034505, 2003.

J. C. Hayes, M. L. Norman, *"Beyond Flux-limited Diffusion: Parallel Algorithms for Multidimensional Radiation Hydrodynamics,"* Astrophysical Journal Supplement Series, **147**, 197-220, 2003.

M. Head-Gordon, T. Van Voorhis, G. Beran and B. Dunietz, *"Local Correlation Models,"* Computational Science: ICCS 2003, Part IV, Lecture Notes in Computer Science, Vol. **2660**, p. 96-102, 2003.

A. Heger, C. L. Fryer, S. E. Woosley, N. Langer, and D. H. Hartmann, *"How Massive Single Stars End Their Life,"* ApJ, **591**:288-300, July 2003.

E. D. Held, *"Unified form for parallel ion viscocus stress in magnetized plasmas,"* Physics of Plasmas, **10**, 4708, 2003.

E. D. Held, J. D. Callen, C. C. Hegna, and C. R. Sovinec, *"Conductive electron heat flow along an inhomogeneous magnetic field,"* Physics of Plasmas **10**, 3933, 2003.

B. Hientzsch, 2003, *"Fast Solvers and Schwarz Preconditioners for Spectral Nedelec Elements for a Model Problem in H(curl),"* Proc of the 14th International Symposium on Domain Decomposition Methods, Cocoyoc, Mexico, Jan. 2002, I. Herrera, D. E. Keyes, O. B. Widlund and R. Yates, eds., 2003.

W. R. Hix, O. E. B. Messer, A. Mezzacappa, M. Liebendoerfer, J. Sampaio, K. Langanke, D. J. Dean, G. Martinez-Pinedo, *"Consequences of Nuclear Electron Capture in Core Collapse Supernovae,"* Physical Review Letters, **91**, 201102, 2003.

W. R. Hix, A. Mezzacappa, O. E. B. Messer, S. W. Bruenn, *"Supernova science at spallation neutron sources,"* Journal of Physics G, **29**, 2523-2542, 2003.

I. Hofmann, G. Franchetti, O. Boine-Frankenheim, J. Qiang, and R. D. Ryne, *"Space-Charge Resonances in Two- and Three-Dimensional Anisotropic Beams,"* Physics Rev. ST Accel. Beams, **6**, 024202, 2003.

I. Hofmann, G. Franchetti, J. Qiang and R. D. Ryne, *"Self-Consistency and Coherent Effects in Nonlinear Resonances,"* Proc. of the 29th ICFA Advanced Beam Dynamics Workshop on Beam Halo Dynamics, Diagnostics, and Collimation (HALO'03), Montauk, NY, May 2003.

M. J. Hogan et al., *"Ultrarelativistic-Positron-Beam Transport through Meter-Scale Plasmas,"* Phys. Rev. Lett. **90**, 205002, 2003.

P. Hovland, K. Keahey, L. C. McInnes, B. Norris, L. Freitag and P. Raghavan, *"A Quality-of-Service Architecture for High-Performance Numerical Components,"* Proceedings of QoSCBSE2003, Toulouse, France, June 2003.

C. Hsu, *"Effects of Block Size on the Block Lanczos Algorithm,"* Senior Thesis, U.C. Berkeley Dept. of Mathematics, June 2003.

P. Hu, N. Chevaugeon, J. E. Flaherty, M. S. Shephard, *"Modelizations of moving object in a fluid flow using level set,"* Proc. 7th US Nat. Congress on Comp. Mech., p. 288, 2003.

A. L. Hungerford, C. L. Fryer, and M. S. Warren, *"Gamma-Ray Lines from Asymmetric Supernovae,"* ApJ, **594**:390-403, Sept. 2003.

M. Ikegami, et al., *"Beam Commissioning of the J-PARC Linac Medium Energy Beam Transport at KEK,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

M. Ikegami, T. Kato, Z. Igarashi, A. Ueno, Y. Kondo, J. Qiang, and R. Ryne, *"Comparison of Particle Simulation with J-PARC Linac MEBT Beam Test Results,"* Proc. of the 29th ICFA Advanced Beam Dynamics Workshop on Beam Halo

Dynamics, Diagnostics, and Collimation (HALO'03), Montauk, NY, May 2003.

J. Ivanic and K. Ruedenberg, *"A MCSCF Method for Ground and Excited States Based on Full Optimizations of Successive Jacobi Rotations,"* Journal of Computational Chemistry, **24**, 1250-1262, 2003.

V. Ivanov, A. Krasnykh, G. Scheitrum, D. Sprehn, L. Ives, G. Miram, *"3D Modeling Activity for Novel High Power Electron Guns at SLAC,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

V. Ivanov, C. Adolphsen, N. Folwell, L. Ge, A. Guetz, Z. Li, C.-K. Ng, G. Schussman, J.W. Wang, M. Weiner, M. Wolf, K. Ko, *"Simulating Accelerator Structure Operation at High Power,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

V. Ivanov, C. Adolphsen, N. Folwell et al., "*Dark Current Simulation and Rise Time Effects at High Power,"* Workshop on High Gradient RF, Chicago, Ill., Oct. 2003.

E. F. Jaeger, L. A. Berry, J. R. Myra, D. B. Batchelor, E. D'Azevedo, P. T. Bonoli, C. K. Phillips, D. N. Smithe, D. A. D'Ippolito, M. D. Carter, R. J. Dumont, J. C. Wright, R. W. Harvey, *"Sheared Poloidal Flow Driven by Mode Conversion in Tokamak Plasmas,"* Physical Review Letters, **90**, 195001, 2003.

A. Jensen, V. Ivanov, A. Krasnykh, G. Scheitrum, *"An Improved Version of TOPAZ3D,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

N. A. C. Johnston, F. S. Rowland, S. Elliott, K. S. Lackner, et al., *"Chemical transport modeling of CO2 sinks,"* Energy Conversion and Management, **44**, 681, 2003.

J. E. Jones, P. S. Vassilevski, and C. S. Woodward, *"Nonlinear Schwarz-FAS Methods for Unstructured Finite Element Problems,"* Proc. of the Second M.I.T. Conference on Computational Fluid and Solid Mechanics, Cambridge, Mass., June 2003.

R. M. Jones, Z. Li, R. H. Miller, T. O. Raubenheimer, *"Optimized Wakefield Suppression & Emittance Dilution-Imposed Alignment Tolerances in X-Band Accelerating Structures for the JLC/NLC,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

G. C. Jordan, S. S. Gupta, B.S. Meyer, *"Nuclear reactions important in alpha-rich freeze-outs,"* Physical Review C, **68**, 065801, 2003.

A. Kabel, *"Maxwell-Lorentz Equations in General Frenet-Serret Coordinates,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

A. Kabel, *"Parallel Simulation Algorithms for the Three-dimensional Strong-Strong Beam-Beam Interaction,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

A. Kabel, *"Particle Tracking and Bunch Population in TRAFIC4 2.0,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

A. Kabel, Y. Cai, B. Erdelyi, T. Sen, and M. Xiao, *"A Parallel Code for Lifetime Simulations in Hadron Storage Rings in the Presence of Parasitic Weak-strong Beam-beam Interactions,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

K. Keahey, *"Fine Grain Authorization Policies in the Grid: Design and Implementation,"* Proc. of the Middleware 2003 Conference, 2003.

E. Kim, J. Bielak, and O. Ghattas, *"Large-scale Northridge Earthquake simulation using octree-based multiresolution mesh method,"* Proc. of 16th ASCE Engineering Mechanics Conference, Seattle, Wash., July 2003.

L. Krivodonova, J. E. Flaherty, *"Error estimation for discontinuous Galerkin solutions of multidimensional hyperbolic problems,"* Advances in Computational Mathematics, 19, 57, 2003.

K. Langanke, D. J. Dean, W. Nazarewicz, *"Shell model Monte Carlo studies of nuclei in the A~80 mass region,"* Nuclear Physics A, **728**, 109-117, 2003.

K. Langanke, G. Martinez-Pinedo, J. M. Sampaio, D. J. Dean, W. R. Hix, O. E. B. Messer, A. Mezzacappa, M. Liebendorfer, H.-T. Janka, M. Rampp, *"Electron Capture Rates on Nuclei and Implications for Stellar Core Collapse,"* Physical Review Letters, **90**, 241102, 2003.

B. S. Lee McCormick, B. Philip, and D. Quinlan, *"Asynchronous fast adaptive composite-grid methods: numerical results,"* SIAM Journal of Scientific Computing, **25**, p. 682-700, 2003.

S. Lefantzi and J. Ray, *"A Component-based Scientific Toolkit for Reacting Flows,"* Computational Fluid and Solid Mechanics, **2**:1401-1405, K. J. Bathe, Ed., Elsevier, 2003.

S. Lefantzi, J. Ray and H. Najm, *"Using the Common Component Architecture to Design High Performance Scientific Simulation Codes,"* Proc. of the Parallel and Distributed Processing Symposium, June 2003.

J. Li, *"A Dual-Primal FETI Method for Solving Stokes/Navier-Stokes Equations,"* Proc of the 14th International Symposium on Domain Decomposition Methods, Cocoyoc, Mexico, Jan. 2002, I. Herrera, D. E. Keyes, O. B. Widlund and R. Yates, eds., 2003.

L. Li, J. Glimm, X. L. Li, *"All isomorphic distinct cases for multi-component interfaces in a block,"* J. Comp. Appl. Mathematics, **152**, p. 263-276, 2003.

X. S. Li and J. W. Demmel, *"SuperLU_DIST: A Scalable Distributed-memory Sparse Direct Solver for Unsymmetric Linear Systems,"* ACM Transactions on Math. Software, **29**:110-140, 2003.

X. Li, M. S. Shephard, M. W. Beall, *"General mesh adaptation using mesh modifications,"* Proc. 7th US Nat. Congress on Comp. Mech., p. 17, 2003.

X. Li, M. S. Shephard, M. W. Beall, *"Accounting for curved domains in mesh adaptation,"* International Journal for Numerical Methods in Engineering, **58**, p. 246-276, 2003.

Z. Li, C. Adolphsen, D. L. Burke, V. Dolgashev, R. M. Jones, R. H. Miller, C. Nantista, C.-K. Ng, T. O. Raubenheimer, R. D. Ruth, P. T. Tenenbaum, J. W. Wang, N. Toge, T. Higo, *"Optimization of the X-band Structure for the JLC/NLC,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

Z. Li, R. Johnson, S. R. Smith, T. Naito, J. Rifkin, *"Cavity BPM with Dipole-mode-selective coupler,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

M. Liebendoerfer, A. Mezzacappa, O. E. B. Messer, G. Martinez-Pinedo, W. R. Hix, F.-K Thielemann, *"The neutrino signal in stellar core collapse and postbounce evolu-*

tion," Nuclear Physics A, **719**, 144-152, 2003.

Y. Lin et al., *"Ion Cyclotron Range of Frequencies Mode Conversion Electron Heating in Deuterium-Hydrogen Plasmas in the Alcator C-Mod Tokamak,"* Plasma Phys. Control. Fusion **45**, (6) 1013, 2003.

Y. Lin, S. J. Wukitch, P. T. Bonoli, A. Mazurenko, E. Nelson-Melby, M. Porkolab, J. C. Wright, I. H. Hutchinson, E. S. Marmar, D. Mossessian, S. Wolfe, C. K. Phillips, G. Schilling, and P. Phillips, *"Study of Ion Cyclotron Range of Frequencies in the Alcator C-Mod Tokamak,"* Radio Frequency Power in Plasmas, Proc. 15th Topical Conf., Moran, Wyoming, 2003.

S. D. Loch, J. P. Colgan, and M. S. Pindzola, M. Westermann, F. Scheuermann, K. Aichele, D. Hathiramani, and E. Salzborn, *"Electron-impact ionization of Oq+ ions for q=1-4,"* Physical Review A, **67**, 042714, 2003.

Y. Luo, I. Malik, Z. Li, M S. Shephard, *"Adaptive mesh refinement in accelerator modeling with OMEGA3P,"* Proc. 7th US Nat. Congress on Comp. Mech., p. 50, 2003.

W. P. Lysenko, J. Qiang, R. W. Garnett, T. P. Wangler, *"Challenge of Benchmarking Simulation Codes for the LANL Beam-Halo Experiment,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

K.-L. Ma, *"Visualizing Time-Varying Volume Data," IEEE Computing in Science and Engineering,"* **5**(2), p. 34, March/April 2003.

M. Macri, S. De, M. S. Shephard, *"Hierarchical tree-based discretization for the method of spheres,"* Computers and Structures, **81**(8-11), p. 789-803, 2003.

G. G. Maisuradze, and D. L. Thompson, *"Interpolating Moving Least-Squares Method for Fitting Potential Energy Surfaces: Illustrative Approaches and Applications,"* Journal of Physical Chemistry A **107**, 7118-7124, 2003.

G. G. Maisuradze, D. L. Thompson, A. F. Wagner, and M. Minkoff, *"Interpolating Moving Least-Squares Method for Fitting Potential Energy Surfaces: Detailed Analysis of One Dimensional Applications,"* Journal of Chemical Physics **119**, 10002-10014, 2003.

T. Manteuffel, S. McCormick, and C. Pflaum, *"Improved discretization error estimates for first-order system least squares (FOSLS),"* Journal on Numerical Analysis, Math., **11**, p. 163-177, 2003.

J. Marathe, F. Mueller, T. Mohan, B. R. de Supinski, S.A. McKee and A. Yoo, *"MET-RIC: Tracking Down Inefficiencies in the Memory Hierarchy Via Binary Rewriting,"* International Symposium on Code Generation and Optimization 2003, San Francisco, Calif., March 2003.

E. S. Marmar, B. Bai, R. L. Boivin, P. T. Bonoli, C. Boswell, R. Bravenec, B. Carreras, D. Ernst, C. Fiore, S. Gangadhara, K. Gentle, J. Goetz, R. Granetz, M. Greenwald, K. Hallatschek, J. Hastie, J. Hosea, A. Hubbard, J. W. Hughes, I. Hutchinson, Y. In, J. Irby, T. Jennings, D. Kopon, G. Kramer, B. LaBombard, W. D. Lee, Y. Lin, B. Lipschultz, J. Liptac, A. Lynn, K. Marr, R. Maqueda, E. Melby, D. Mikkelsen, D. Mossessian, R. Nazikian, W. M. Nevins, R. Parker, T. S. Pedersen, C. K. Phillips, P. Phillips, C. S. Pitcher, M. Porkolab, J. Ramos, M. Redi, J. Rice, B. N. Rogers, W. L. Rowan, M. Sampsell, G. Schilling, S. Scott, J. Snipes, P. Snyder, D. Stotler, G. Taylor, J. L. Terry, H. Wilson, J. R. Wilson, S. M. Wolfe, S. Wukitch, X. Q. Xu, B. Youngblood, H. Yuh, K. Zhurovich and S. Zweben, *"Overview of recent Alcator C-Mod research,"* Nucl. Fusion **43**, 1610, 2003.

G. Martinez-Pinedo, D. J. Dean, K. Langanke, J. Sampaio, *"Neutrino-nucleus interactions in core-collapse supernova,"* Nuclear Physics A, 718, 452-454, 2003.

W. Maslowski, and W. H. Lipscomb, *"High-resolution simulations of Arctic sea ice during 1979-93,"* Polar Research, **22**, 67, 2003.

L. McInnes, B. Norris, S. Bhowmick, and P. Raghavan, 2002, *"Adaptive Sparse Linear Solvers for Implicit CFD Using Newton-Krylov Algorithms,"* Proc. of the Second MIT Conference on Computational Fluid and Solid Mechanics, Boston, Mass., June 2003.

D. J. McGillicuddy, L. A. Anderson, S. C Doney and M. E. Maltrud, *"Eddy-driven sources and sinks of nutrients in the upper ocean: results from a 0.1 degree resolution model of the North Atlantic,"* Global Biogeochemical Cycles, **17**, 1035, 2003.

O. E. B. Messer, W. R. Hix, M. Liebendorfer, A. Mezzacappa, *"Electron capture and shock formation in core-collapse supernovae,"* Nuclear Physics, A. **718**, 449-451, 2003.

O. E. B. Messer, M. Liebendorfer, W. R. Hix, A. Mezzacappa, S. W. Bruenn, *"The Impact of Improved Weak Interaction Physics in Core-Collapse Supernova Simulations,"* From Twilight to Highlight: The Physics of Supernovae, W. Hillebrandt, D. Leibundgut, eds., p. 70, Springer-Verlag, 2003.

B. S. Meyer, *"Neutrinos, supernovae, molybdenum, and extinct 92Nb,"* Nuclear Physics A, **719**, 13-20, 2003.

A. Mezzacappa, *"The Road to Prediction: Toward Gravitational Wave Signatures from Core Collapse Supernovae,"* AIP Conf. Proc. 686: The Astrophysics of Gravitational Wave Sources, p. 29-39, 2003.

A. Mezzacappa, J. M. Blondin, *"A New Twist on the Core Collapse Supernova Mechanism?"* in From Twilight to Highlight: The Physics of Supernovae, W. Hillebrandt, D. Leibundgut, eds., p. 63, Springer-Verlag, 2003.

D. Mika, P. Myers, A. Majorell, L. Jiang, S. Kocak, J. Wan, M. S. Shephard, *"Alloy 718 extrusion modeling - unstable flow and mesh enrichment,"* Proc. 7th US Nat. Congress on Comp. Mech., p. 342, 2003.

A. J. Miller, M. A. Alexander, G. J. Boer, F. Chai, K. Denman, D. J. Erickson III, R. Frouin, A. Gabric, E. Laws, M. Lewis, Z. Liu, R. Murtugudde, S. Nakamoto, D. J. Neilson, J. R. Norris, C. Ohlmann, I. Perry, N. Schneider, K. Shell and A. Timmermann, *"Potential feedbacks between Pacific Ocean ecosystems and interdecadel climate variations,"* Bulletin of the American Meteorology, Soc. **84**, 617, 2003.

G. H. Miller, *"An iterative Riemann solver for systems of hyperbolic conservation laws, with application to hyperelastic solid mechanics,"* Journal of Computational Physics **193**, p. 198-225, 2003.

D. M. Mitnik, D. C. Griffin, C. P. Ballance, and N. R. Badnell, *"An R-matrix with pseudo-states calculation of electron-impact excitation in C^{2+},"* Journal of Physics B, **36**, 717, 2003.

T. Mohan, B. R. de Supinski, S. A. McKee, F. Mueller, A. Yoo, M. Schulz, *"Identifying and Exploiting Spatial Regularity in Data Memory References,"* Proc. of ACM/IEEE SC03 conference, Phoenix, Ariz., Nov. 2003.

J. Mueller, S. Nagrath, X. Li, J. E. Jansen, M. S. Shephard, *"Efficient computational methods for the investigation of vascular disease,"* Proc. 7th US Nat. Congress on Comp. Mech., p. 195, 2003.

J. D. Myers, C. Pancerella, C. Lansing, K. L. Schuchardt and B. Didier, *"Multi-scale science: Supporting emerging practice with semantically-derived provenance,"* Proc. of the Workshop on Semantic Web Technologies for Searching and Retrieving Scientific Data, Sanibel Island, Fla., Oct. 2003.

J. D. Myers, A. Chappell, M. Elder, A. Geist, J. Schwidder, *"Re-integrating the research record,"* IEEE Computing in Science and Engineering, **5**(3):44-50, 2003.

D. Narayan, R. Bradshaw, R. Evard and A. Lusk, *"Bcfg: a configuration management tool for heterogeneous environments,"* Proc. of the 5th IEEE International Conference on Cluster Computing (CLUSTER03), Kowloon, Hong Kong, Dec. 2003.

E. Nelson-Melby, M. Porkolab, P. T. Bonoli, Y. Lin, A. Mazurenko, and S. J. Wukitch, *"Experimental Observations of Mode-Converted Ion Cyclotron Waves in a Tokamak Plasma by Phase Contrast Imaging,"* Physical Review Letters, **90**, 155004, 2003.

R. M. Olson, M. W. Schmidt, M. S. Gordon and A. P. Rendell, *"Enabling the Efficient Use of SMP Clusters: The GAMESS/DDI Model,"* Proc. of the ACM/IEE SC03 conference, Phoenix, Ariz., Nov. 2003.

E. Ong, J. Larson and R. Jacob, *"A Real Application of the Model Coupling Toolkit,"* Proc. of the 2002 International Conference on Computational Science, eds. P. Sloot, C. J. K. Tan, J. J. Dongarra, A. Hoekstra, Springer-Verlag, 2003.

C. M. Pancerella, J. Hewson, W. Koegler D. Leahy, M. Lee, L. Rahn, C. Yang, J. D. Myers, D. Didier, R. McCoy, *"Metadata in the collaboratory for multi-scale chemical science,"* Proc, of the 2003 Dublin Core Conference: Supporting Communities of Discourse and Practice-Metadata Research and Applications, Seattle, Wash., Sept.-Oct. 2003.

W. Park, J. Breslau, J. Chen, et al,, *"Nonlinear simulation studies of tokamaks and STs,"* Nuclear Fusion **43**, 483, 2003.

M. S. Pindzola, T. Minami, and D. R. Schultz, *"Laser-modified charge-transfer processes in proton collisions with lithium atoms,"* Physical Review A, **68**, 013404, 2003.

M. S. Pindzola and F. Texier, *"Collective modes of ground and dark-soliton states of Bose-Einstein condensates in anisotropic traps,"* Journal of Physics B, **36**, 1783, 2003.

A. Pochinsky, et al., *"Large scale commodity clusters for lattice QCD,"* Nuclear Physics B (Proc. Suppl.) **119**, 1044, 2003.

J. Pruet, *"Neutrinos from the Propagation of a Relativistic Jet through a Star,"* ApJ, **591**:1104-1109, July 2003.

J. Pruet and G. M. Fuller, *"Estimates of Stellar Weak Interaction Rates for Nuclei in the Mass Range A=65-80,"* Astrophysical Journal Supplement, **149**:189-203, Nov. 2003.

J. Pruet, S. E. Woosley, and R. D. Hoffman, *"Nucleosynthesis in Gamma-Ray Burst Accretion Disks,"* ApJ, **586**:1254-1261, April 2003.

J. Qiang and R. W. Garnett, *"Smooth Approximation with Acceleration in an Alternating Phase Focusing Superconducting Linac,"* Nuclear Instruments and Methods in Physics Res. A **496**, 33, 2003.

J. Qiang, M. Furman and R. Ryne, *"Parallel Particle-In-Cell Simulation of Colliding Beams in High Energy Accelerators,"* Proc. of the ACM/IEEE SC03 conference, Phoenix, Ariz., Nov. 2003.

J. Qiang, M. Furman, R. D. Ryne, W. Fischer, T. Sen, M. Xiao, *"Parallel Strong-Strong/Strong-Weak Simulations of Beam-Beam Interactions in Hadron Accelerators,"* Proc. of the 29th ICFA Advanced Beam Dynamics Workshop on Beam Halo Dynamics, Diagnostics, and Collimation (HALO'03), Montauk, NY, May 2003.

J. Qiang, R. D. Ryne, and I. Hofmann, *"Space-Charge Driven Emittance Growth in a 3D Mismatched Anisotropic Beam,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

J. Qiang, R. D. Ryne, T. Sen, M. Xiao, *"Macroparticle Simulations of Antiproton Lifetime at 150 GeV in the Tevatron,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

D. Quinlan and M. Schordan, *"A Source-to-Source Architecture for User-Defined Optimizations,"* Joint Modular Languages Conference, Austria, Lecture Notes in Computer Science, **2789**, p. 214-223, Springer-Verlag, Aug. 2003.

D. Quinlan, M. Schordan, B. Miller and M. Kowarschik, *"Parallel Object-Oriented Framework Optimization,"* Special Issue of Concurrency: Practice and Experience, **16**, 2-3, p. 293-302, 2003.

D. Quinlan, M. Schordan, Q. Yi, and B. R. de Supinski, *"Semantic-driven Parallelization of Loops Operating on User-Defined Containers,"* 16th Annual Workshop on Languages and Compilers for Parallel Computing, College Station, Texas, Oct. 2003.

D. Quinlan, M. Schordan, Qing Li, and B. R. de Supinski, *"A C++ Infrastructure for Automatic Introduction and Translation of OpenMP Directives,"* Proc. of the Workshop on Open MP Applications and Tools (WOMPAT'03), Lecture Notes in Computer Science, 2716, p. 13-25, Springer-Verlag, June 2003.

P. Raghavan, K. Teranishi, and E. G. Ng, *"A Latency Tolerant Hybrid Sparse Solver Using Incomplete Cholesky Factorization,"* Numerical Linear Algebra with Applications **10**, p. 541-560, 2003.

S. Ratkovic, S. Iyer Dutta, M. Prakash, *"Differential neutrino rates and emissivities from the plasma process in astrophysical systems,"* Physical Review D, **67**, 123002, 2003.

D. A. Reed, C. L. Mendes and C. Lu, *"Intelligent Application Tuning and Adaptation,"* Chapter in The Grid: Blueprint for a New Computing Infrastructure, 2nd edition, I. Foster & C. Kesselman eds., Morgan Kaufmann, Nov. 2003.

D. A. Reed, C. Lu, C. L. Mendes, *"Big Systems and Big Reliability Challenges,"* Proc. of Parallel Computing 2003, Dresden, Germany, Sept. 2003. J. F. Remacle, J. E. Flaherty, M. S. Shephard, "An adaptive discontinuous Galerkin technique with an orthogonal basis applied compressible flow problems," SIAM Review, **45**(1), p. 53-72, 2003.

J. F. Remacle, M. S. Shephard, *"An algorithm oriented mesh database,"* International Journal for Numerical Methods in Engineering, **58**, p. 349-374, 2003.

J. Rikovska Stone, J. C. Miller, R. Koncewicz, P. D. Stevenson, M. R. Strayer,

"Nuclear matter and neutron-star properties calculated with the Skyrme interaction," Physical Review C, **68**, 034324, 2003.

F. J. Robicheaux and J. D. Hanson, *"Simulated expansion of an ultracold neutral plasma,"* Physics of Plasmas, **10**, 2217, 2003.

T. M. Rogers, G. A. Glatzmaier, and S. E. Woosley, *"Simulations of two-dimensional turbulent convection in a density-stratified fluid,"* Physical Review E, **67**(2):026315, Feb. 2003.

G. Rosa, E. Lum, K.-L. Ma, and K. Ono, *"An Interactive Volume Visualization System for Transient Flow Analysis,"* Proc. of the Volume Graphics 2003 Workshop, Tokyo, Japan, July 2003.

A. L. Rosenberg, J. E. Menard, J. R. Wilson, S. Medley, R. Andre, D. Darrow, R. Dumont, B. P. LeBlanc, C. K. Phillips, M. Redi, T. K. Mau, E. F. Jaeger, P. M. Ryan, D. W. Swain, R. W. Harvey, J. Egedal, and the NSTX Team, *"Characterization of Fast Ion Absorption of the High Harmonic Fast Wave in the National Spherical Torus Experiment,"* Radio Frequency Power in Plasmas, Proc. 15th Topical Conf., Moran, Wyoming, AIP, N. Y., 185, 2003.

G. Rumolo, A. Z. Ghalam, et al., *"Electron Cloud Effects on Beam Evolution in a Circular Accelerator,"* Phys. Rev. STAB, **6**, 081002, 2003.

J. M. Sampaio, K. Langanke, G. Martinez-Pinedo, E. Kolbe, D. J. Dean, *"Electron capture rates for core collapse supernovae,"* Nuclear Physics A, **718**, 440-442, 2003.

R. Samtaney, *"Suppression of the Richtmyer-Meshkov instability in the presence of a magnetic field,"* Physics of Fluids **15**, L53-56, 2003.

S. Sankaran, J. M. Squyres, B. Barrett, A. Lumsdaine, J. Duell, P. Hargrove and E. Roman, *"The LAM/MPI Checkpoint/Restart Framework: System-Initiated Checkpointing,"* LACSI Symposium, Santa Fe, NM, Oct. 2003.

D. P. Schissel, *"National Fusion Collaboratory - Advancing the Science of Fusion Research,"* Proc. of the 2003 DOE SciDAC PI Meeting, 2003.

M. Schnell, G. Gwinner, N. R. Badnell, M. E. Bannister, S. Bohm, J. P. Colgan, S. Kieslich, S. D. Loch, D. Mitnik, A. Muller, M. S. Pindzola, S. Schippers, D. Schwalm, W. Shi, A. Wolf and S. G. Zhou, *"Observation of trielectronic recombination in Be-like Cl ions,"* Physical Review Letters, **91**, 043001, 2003.

M. Schordan and D. Quinlan, *"A Source-to-Source Architecture for User-Defined Optimizations,"* Proc, of the Joint Modular Languages Conference (JMLC'03), Lecture Notes in Computer Science, **2789**, p. 214-223, Springer-Verlag, June 2003.

D. R. Schultz and P. S. Krstic, *"Ionization of Helium by antiprotons: Fully correlated, four-dimensional lattice approach,"* Physical Review A, 022712, 2003.

G. L. Schussman, *"Interactive And Perceptually Enhanced Visualization Of Large, Complex Line-Based Datasets,"* Ph.D. thesis, University of California Davis. Dec. 2003.

S. L. Scott, B. Luethke and J. Mugler, *"Cluster & Grid Tools: C3 Power Tools with C2G,"* Newsletter of the IEEE Task Force on Cluster Computing, **4,** 2, March/April 2003.

S. L. Scott, C. Leangsuksun, L Chen and T. Lui, *"Building High Availability and Performance Clusters with HA-OSCAR Toolkits,"* 2003 High Availability and Performance Workshop, Santa Fe, NM, Oct. 2003.

S. L. Scott, C. Leangsuksun, L. Shen, T. Liu and H. Song, *"Availability Prediction and Modeling of High Availability OSCAR Cluster,"* Proc. of the 5th IEEE International Conference on Cluster Computing (CLUSTER03), Kowloon, Hong Kong, Dec. 2003.

S. L. Scott, B. Luethke and T. Naughton, *"OSCAR Cluster Administration With C3,"* Proc. of the 17th Annual International Symposium on High Performance Computing Systems and Applications and the 1st Annual OSCAR Symposium, Quebec, Canada, May 2003.

S. L. Scott, C. Leangsuksun, L. Shen, H. Song and I. Haddad, *"The Modeling and Dependability Analysis of High Availability OSCAR Cluster System,"* Proc. of the 17th Annual International Symposium on High Performance Computing Systems and Applications and the 1st Annual OSCAR Symposium, Quebec, Canada, May 2003.

S. L. Scott, T. Naughton, B. Ligneris and N. Gorsuch, *"Open Source Cluster Application Resources (OSCAR): Design, Implementation and Interest for the [Computer] Scientific Community,"* Proc. of the 17th Annual International Symposium on High Performance Computing Systems and Applications and the 1st Annual OSCAR Symposium, Quebec, Canada, May 2003.

S. L. Scott, B. Luethke, *"Scalable C3 Power Tools,"* Cluster World Conference and Expo (CWCE 2003) and 4th Linux Cluster Institute Conference (LCI), San Jose, Calif., June 2003.

S. L. Scott, J. Mugler, T. Naughton, B. Barrett, A. Lumsdaine, J. Squyres, B. Ligneris, F. Giraldeau and C. Leangsuksun, *"OSCAR Clusters,"* Proc. of the Ottawa Linux Symposium (OLS'03), Ottawa, Canada, July 2003.

S. L. Scott, C. Leangsuksun, L. Shen, T. Liu and H. Song, *"Dependability Prediction of High Availability OSCAR Cluster Server,"* 2003 International Conference on Parallel and Distributed Processing Techniques and Applications (PDPTA'03), Las Vegas, Nevada, June 2003.

S. L. Scott, I. Haddad and C. Leangsuksun, *"HA-OSCAR: The birth of a Highly Available OSCAR,"* Linux Journal, **2003**, 115, Seattle, Wash., Nov. 2003.

S. L. Scott, T. Naughton, Y. C. Fang, P. Pfeiffer, B. Ligneris, and C. Leangsuksun, *"The OSCAR Toolkit: Current and Future Developments,"* Dell Power Solution magazine, Nov. 2003.

S. L. Scott, T. Naughton, B. Barrett, J. Squyres, A. Lumsdaine, Y. C. Fang, and V. Mashayekhi *"Looking Inside the OSCAR Cluster Toolkit,"* Dell Power Solution magazine, Nov. 2003.

A. Snavely, L. Carrington, N. Wolter, C. Lee, J. Labarta, J. Gimenez, and P. Jones, *"Performance Modeling of HPC Applications, Mini-symposium on Performance Modeling,"* Proc. of Parallel Computing 2003, Dresden, Germany, Sept. 2003.

C. Sneden, J. J. Cowan, J. E. Lawler, I. I. Ivans, S. Burles, T. C. Beers, F. Primas, V. Hill, J. W. Truran, G. M. Fuller, B. Pfeiffer, K.-L. Kratz, *"The Extremely Metal-poor, Neutron Capture-rich Star CS 22892-052: A Comprehensive Abundance Analysis,"* Astrophysical Journal Letters, **591**, 936-953, 2003.

C. R. Sovinec, T. A. Gianakon, E. D. Held, S. E. Kruger, D. D. Schnack and the NIMROD Team, *"NIMROD: a computa-*

tional laboratory for studying nonlinear fusion magnetohydrodynamics," Physics of Plasmas **10**, 1727, 2003.

C. R. Sovinec, B. I. Cohen, G. A. Cone, E. B. Hooper, and H. S. McLean, *"Numerical investigation of transients in the SSPX spheromak,"* Physical Review Letters **94**, 035003, 2003.

P. Spentzouris, J. Amundson, *"FNAL Booster: experiment and modeling,"* Proc. of IEEE Particle Accelerator Conference 2003, Portland, Ore., May 2003.

N. Stojic, J. W. Davenport, M. Komelj, J. Glimm, *"Surface magnetic moment in \alpha-uranium by density-functional theory,"* Phys. Rev. B, **68**, 094407, 2003.

P. H. Stoltz, M. A. Furman, J. -L. Vay, A. W. Molvik, R. H. Cohen, *"Numerical Simulation of the Generation of Gecondary Electrons in the High Current Experiment,"* Physics Rev. ST Accel. Beams. Vol **6**, 054701. 2003.

A. Stompel, K.-L. Ma, J. Bielak, O. Ghattas and E. Kim, *"Visualizing Large-Scale Earthquake Simulations,"* Proc. of the ACM/IEEE SC03 conference, Phoenix, Ariz., Nov. 2003.

A. Stompel, K.-L. Ma, E. Lum, J. Ahrens, and J. Patchett, *"SLIC: Scheduled Linear Image Compositing for Parallel Vollume Rendering,"* Proc. of the 2003 Symposium on Parallel Visualization and Graphics, Seattle, WA, Oct. 2003.

D. W. Swain, M. D. Carter, J. R. Wilson, P. M. Ryan, J. B. Wilgen, J. Hosea and A. Rosenberg, *"Loading and Asymmetry Measurements and Modeling for the National Spherical Torus Experiment Ion Cyclotron Range of Frequencies System,"* Fusion Science and Technology, **43**, 503, 2003.

K. Takahashi, K. Sato, A. Burrows, and T. Thompson, *"Supernova neutrinos, neutrino oscillations, and the mass of the progenitor star,"* Phys. Rev. D, **68**:113009, 2003.

T. J. Tautges, *"MOAB-SD: Integrated Structured and Unstructured Mesh Representation,"* 6th U.S. Congress on Computational Mechanics, Trends in Unstructured Mesh Generation, Albuquerque, NM, July 2003.

F.-K. Thielemann, D. Argast, F. Brachwitz, W. R. Hix, P. Hoflich, M. Liebendorfer, G. Martinez-Pinedo, A. Mezzacappa, I. Panov, T. Rauscher, *"Nuclear cross sections, nuclear structure and stellar nucleosynthesis,"* Nuclear Physics A, **718**, 139-146, 2003.

F.-K. Thielemann, D. Argast, F. Brachwitz, W. R. Hix, P. Hoflich, M. Liebendorfer, G. Martinez-Pinedo, A. Mezzacappa, K. Nomoto, I. Panov, I. *"Supernova Nucleosynthesis and Galactic Evolution,"* From Twilight to Highlight: The Physics of Supernovae, W. Hillebrandt, D. Leibundgut, eds., p. 331, Springer-Verlag, 2003.

S. J. Thomas, J. M. Dennis, H. M. Tufo, P. F. Fischer, *"A Schwarz Preconditioner for the Cubed-Sphere,"* SIAM J. Sci. Comp., **25**, p. 442-453, 2003.

M. Thompson, *"Fine-grained Authorization for Job and Resource Management using Akenti and Globus,"* Proceedings of the 2003 Conference for Computing in High Energy and Nuclear Physics, 2003.

T. A. Thompson, A. Burrows, and P. A. Pinto, *"Shock Breakout in Core-Collapse Supernovae and Its Neutrino Signature,"* Astrophysical Journal, **592**:434-456, July 2003.

C. Tse, S. T. Teoh, and K.-L. Ma, *"An Interactive Isosurface Visualization Cluster,"* Proc. of High Performance Computing 2003 Symposium, Orlando, Fla., March 2003.

M. Valorani, F. Creta and D. A. Goussis, *"Local and Global Manifolds in Stiff Reaction-Diffusion Systems,"* Computational Fluid and Solid Mechanics 2003, 1548-1551, K. J. Bathe, ed., Elsevier, 2003.

M. Valorani, H. N. Najm and D. A. Goussis, *"CSP Analysis of a Transient Flame-Vortex Interaction: Time Scales and Manifolds,"* Combustion and Flame, **134**(1-2):35-53, July 2003.

J. S. Vetter and F. Mueller, *"Communication Characteristics of Large-Scale Scientific Applications for Contemporary Cluster Architectures,"* Journal of Parallel and Distributed Computing, **63**, p. 853-865, 2003.

R. Vuduc, *"Automatic Performance Tuning of Sparse Matrix Kernels,"* Ph.D. thesis, U.C. Berkeley Dept. of Computer Science, Dec. 2003.

R. Vuduc, A. Gyulassy, J. W. Demmel and K. A. Yelick, *"Memory Hierarchy Optimizations and Performance Bounds for Sparse ATA*x,"* Proc. of ICCS 2003: Workshop on Parallel Linear Algebra, Melbourne, Australia, June 2003.

G. Wallace, et al., *"DeskAlign: Automatically Aligning a Tiled Windows Desktop,"* Proc. of the IEEE International Workshop on Projector-Camera Systems (PROCAMS), Oct. 2003.

G. Wallace, et al., *"Color Gamut Matching for Tiled Display Walls,"* Proc. of the Immersive Projection Technology Workshop (IPT), May 2003.

J. Wan, S. Kocak, M. S. Shephard, *"Automated adaptive forming simulations,"* 12th International Meshing Roundtable, Sandia National Laboratories, p. 323-334, 2003.

J. Wan, S. Kocak, M. S. Shephard, *"Controlled mesh enrichments for evolving geometries,"* Proc. 7th US Nat. Congress on Comp. Mech., p. 42, 2003.

T. P. Wangler, K. R. Crandall, R. W. Garnett, D. Gorelov, P. Ostroumov, J. Qiang, R. Ryne, R. York, *"Advanced Beam-Dynamics Simulation Tools for the RIA Driver Linac, Part I: Low Energy Beam Transport and Radiofrequency Quadrupole,"* Proc. RIA R&D Workshop, Washington, D.C., Aug. 2003.

A. Wetzels, A. Gurtler, F. Rosca-Pruna, S. Zamith, M. J. J. Vrakking, F. Robicheaux and W. J. van der Zande, *"Two-dimensional momentum imaging of Rydberg states using half-cycle pulse ionization and velocity map imaging,"* Physical Review A, **68**, 041401, 2003.

M. Wingate, et al. (The HPQCD Collaboration), "*Bs Mesons Using Staggered Light Quarks,"* Nuclear Physics B (Proc. Suppl.) **119**, 604, 2003.

M. C. Witthoeft, J. P. Colgan, and M. S. Pindzola, *"Electron-impact excitation of Li to high principal quantum number,"* Physical Review A, **68**, 022711, 2003.

F. Wolf, B. Mohr, *"Automatic performance analysis of hybrid MPI/OpenMP applications,"* Journal of Systems Architecture, Special Issue: Evolutions in Parallel Distributed and Network-Based Processing, A. Clematis, D. D'Agostino, eds., Elsevier, **49**(10-11), p. 421-439, Nov. 2003.

P. H. Worley, T. H. Dunigan, *"Early Evaluation of the Cray X1 at Oak Ridge National Laboratory,"* Proc. of the 45th Cray User Group Conference, Columbus, Ohio, May 2003.

J. C. Wright, P. T. Bonoli, M. Brambilla, F. Meo, E. D'Azevedo, D. B. Batchelor, E. F. Jaeger, L. A. Berry, C. K. Phillips and A. Pletzer, *"Full Wave Simulations of Fast*

Wave Mode Conversion and Lower Hybrid Wave Propagation in Tokamaks," Bull. Am. Phys. Soc. **48**, 127, 2003.

K. Wu, W. Koegler, J. Chen and A. Shoshani, *"Using bitmap index for interactive exploration of large datasets,"* Proc. of SSDBM 2003, p. 65, Cambridge, Mass, USA, 2003.

K. Wu, W.-M. Zhang, A. Sim, J. Gu and A. Shoshani, *"Grid collector: An event catalog with automated file management,"* Proc. of IEEE Nuclear Science Symposium 2003, 2003.

R. G. Zepp, T. V. Callaghan and D. J. Erickson III, *"Interactive effects of ozone depletion and climate change on biogeochemical cycles,"* Journal of Photochemistry, Photobiol. **2**, 51, 2003.

O. Zatsarinny, T. W. Gorczyca, K. T. Korista, N. R. Badnell and D. W. Savin, *"Dielectronic recombination data for dynamic finite-density plasmas: II. The Oxygen isoelectronic sequence,"* Astronomy and Astrophysics, **412**, 587, 2003.

M. Zeghal, U. El Shamy, M. S. Shephard, R. Dobry, J. Fish, T. Abdounm, *"Micromechanical analysis of saturated granular soils,"* Journal of Multiscale Computational Engineering, **1**(4), p. 441-460, 2003.

W. Zhang, S. E. Woosley, and A. I. MacFadyen, *"Relativistic Jets in Collapsars,"* Astrophysical Journal, **586**:356-371, March 2003.

2004

A. Adelmann, J. Amundson, P. Spentzouris, J. Qiang, R. D. Ryne, *"A Test Suite of Space-charge Problems for Code Benchmarking,"* Proc. of EPAC 2004, Lucerne, Switzerland, p. 1942, 2004.

P. K. Agarwal, R. A. Alexander, E. Apra, S. Balay, A. S. Bland, J. Colgan, E. F. D'Azevedo, J. J. Dongarra, T. H. Dunigan, Jr., M. R. Fahey, R. A. Fahey, A. Geist, M. Gordon, R. J. Harrison, D. Kaushik, M. Krishnakumar, P. Lusczek, A. Mezzacappa, J. A. Nichols, J. Nieplocha, L. Oliker, T. Packwood, M. S. Pindzola, T. C. Shulthess, J. S. Vetter, J. B. White III, T. L. Windus, P. H. Worley, T. Zacharia, *"ORNL Cray X1,"* Proc. of the 46th Cray User Group Conference, Knoxville, TN, May 2004.

V. Akcelik, J. Bielak, G. Biros, I. Epanomeritakis, O. Ghattas, L. Kallivokas and E. Kim, *"An Online Framework for Inversion-Based 3D Site Characterization,"* Lecture Notes in Computer Science, **3038**, p. 717, Springer-Verlag, 2004.

M. A. Albao, D.-J. Liu, C. H. Choi, M. S. Gordon and J. W. Evans, *"Atomistic modeling of morphological evolution during simultaneous etching and oxidation of Si(100),"* Surface Science **555**, 51, 2004.

A. Alexakis, A. C. Calder, A. Heger, E. F. Brown, L. J. Dursi, J. W. Truran, R. Rosner, D. Q. Lamb, F. X. Timmes, B. Fryxell, M. Zingale, P. M. Ricker and K. Olson, *"On Heavy Element Enrichment in Classical Novae,"* ApJ, **602**:931-937, Feb. 2004.

C. Alexandru, et al., *"N to Delta electromagnetic transition form factors from lattice QCD,"* Physical Review D, **69**, 114506, 2004.

C. Alexandrou, et al., *"gamma N – Delta transition form factors in quenched and N(F) = 2 QCD,"* Nuclear Physics (Proc. Suppl.) 129-130, **302**, 2004.

J. Amundson, P. Spentzouris, *"Emittance dilution and halo creation during the first milliseconds after injection at the Fermilab Booster,"* Proc. 33rd ICFA Advanced Beam Dynamics Workshop on High Intensity & High Brightness Hadron Beams, Bensheim, Germany, Oct. 2004.

J. Amundson, P. Spentzouris, J. Qiang, R. D. Ryne, A. Adelmann, *"A test suite of space-charge problems for code benchmarking,"* 9th European Particle Accelerator Conference (EPAC 2004), Lucerne, Switzerland, July 2004.

A. Andrady, P. J. Aucamo, A. F. Bais, C. L. Ballare, L. O. Bjorn, J. F. Bornman, M. Caldwell, A. P. Cullen, D. J. Erickson III, F. R. de Gruijl, D.-P. Hader, M. ilyas, G. Kulandaivelu, H. D. Kumar, J. Longstreth, R. L. McKenzie, M. Norval, H. H. Redhwi, R. C. Smith, K. R. Solomon, Y. Takizawa, X. Tang, A. H. Teramura, A. Torikai, J. C. van der Leun, S. Wilson, R. C. Worrest, and R. G. Zepp, *"Environmental effects of ozone depletion and its interactions with climate change: Progress Report 2003,"* Photochemical and Photobiological Sciences. **3**, 1-5, 2004.

C. Aubin, et al. (The HPQCD, MILC and UKQCD Collaborations), *"First determination of the strange and light quark masses from full lattice QCD,"* Physical Review D, **70**, 031504(R), 2004.

C. Aubin, et al. (The MILC Collaboration), *"Light hadrons with improved staggered quarks: approaching the continuum limit,"* Physical Review D **70**, 094505, 2004.

C. Aubin, et al. (The MILC Collaboration), *"Light pseudoscalar decay constants, quark masses, and low energy constants from three-flavor lattice QCD,"* Physical Review D, **70**, 114501, 2004.

C. Aubin, et al. (The MILC Collaboration), *"Pion and kaon physics with improved staggered quarks,"* Nuclear Physics B (Proc. Suppl.), 129-130, **227**, 2004.

T. Austin, T. Manteuffel, and S. McCormick, *"A robust approach to minimizing H(div) dominated functionals in an H1-conforming finite element space,"* Journal on Numerical Analysis, Lin. Alg. App. **11**, p. 115, 2004.

I. Baraffe, A. Heger, and S. E. Woosley, *"Stability of Supernova Ia Progenitors against Radial Oscillations,"* ApJ, **615**:378-382, Nov. 2004.

S. Basak, et al. (The LHPC Collaboration), *"Baryon operators and spectroscopy in lattice QCD,"* Nuclear Physics (Proc. Suppl.) 129-130, **186**, 2004.

S. Basak, et al. (The LHPC Collaboration), *"Mass spectrum of N* and source optimization,"* Nuclear Physics (Proc. Suppl.) 129-130, **209**, 2004.

D. B. Batchelor, E. F. Jaeger, L. A. Berry, E. D'Azevedo, M. D. Carter, R. W. Harvey, R. J. Dumont, J. R. Myra, A. A. D'Ippolito, D. N. Smithe, C. K. Phillips, P. T. Bonoli and J. C. Wright, *"Integrated modeling of wave-plasma interactions in fusion systems,"* Theory of Fusion Plasmas, Proc. of the Joint Varenna-Lausanne International Workshop Varenna, Italy, Aug.-Sept. 2004.

M. W. Beall, J. Walsh, M. S. Shephard, *"A comparison of techniques for geometry access related to mesh generation,"* Engineering with Computers, **20**(3), p. 210-221, 2004.

J. B. Bell, M. S. Day, C. A. Rendleman, S. E. Woosley, and M. A. Zingale, *"Direct Numerical Simulations of Type Ia Supernovae Flames II: The Rayleigh-Taylor Instability,"* Astrophysical Journal, **608**, 883, 2004.

J. B. Bell, M. S. Day, C. A. Rendleman, S. E. Woosley, and M. A. Zingale, *"Direct Numerical Simulations of Type Ia Supernovae Flames I: The Landau-Darrieus Instability,"* Astrophysical Journal, **606**, 1029, 2004.

J. B. Bell, M. S. Day, C. A. Rendleman, S. E. Woosley, and M. A. Zingale, *"Adaptive low Mach number simulations of nuclear flame microphysics,"* Journal of Computational Physics, **195**:677-694, April 2004.

J. B. Bell, M. S. Day, J. F. Grcar, and M. J. Lijewski, *"Stochastic Algorithms for the Analysis of Numerical Flame Simulations,"* Journal of Computational Physics, **202**, 262, 2004.

S. Belviso, L. Bopp, C. Moulin, J. C. Orr, T. R. Anderson, O. Aumont, S. Chu, S. Elliott, M. E. Maltrud and R. Simó, *"Comparison of global climatological maps of sea surface dimethylsulfide,"* Global Biogeochemical Cycles, **18**(3), GB3013, 2004.

S. J. Benson, L. Curfman McInnes, J. J. Moré and J. Sarich, *"Scalable Algorithms in Optimization: Computational Experiments,"* AIAA Multidisciplinary Analysis and Optimization Conference, 2004.

G. J. O. Beran and M. Head-Gordon, *"Extracting dominant pair correlations from many-body wavefunctions,"* Journal of Chemical Physics, **121**, 78-88, 2004.

C. Bernard, et al. (The MILC Collaboration), *"Quark Loop Effects in Semileptonic Form Factors for Heavy-Light Mesons,"* Nuclear Physics B (Proc. Suppl.), 129-130, **364**, 2004.

C. Bernard, et al. (The MILC Collaboration), *"The Phase Diagram of High Temperature QCD with Three Flavors of Improved Staggered Quarks,"* Nuclear Physics B (Proc. Suppl.), 129-130, **626**, 2004.

C. Bernard, et al. (The MILC Collaboration), *"Excited States in Staggered Meson Propagators,"* Nuclear Physics B (Proc. Suppl.), 129-130, **230**, 2004.

S. Bhowmick, P. Raghavan, L. McInnes, and B. Norris, *"Faster PDE-based Simulations Using Robust Composite Linear Solvers,"* Future Generation Computer Systems, The International Journal of Grid Computing: Theory, Methods and Applications, **20**, p. 373-387, 2004.

B. Billeter, C. DeTar, and J. Osborn, *"Topological susceptibility in staggered fermion chiral perturbation theory,"* Physical Review D, **70**, 077502, 2004.

L. Bonaventura, and T. D. Ringler, *"Analysis of discrete shallow-water models on geodesic Delaunay grids with C-type staggering,"* Monthly Weather Review, **133**, 2351, 2004.

P. T. Bonoli et al., *"Full-wave Electromagnetic Field Simulations in the Lower-Hybrid Range of Frequencies,"* Bull. American Phys. Soc. **49**, 325, RI13, 2004.

M. Brezina, R. Falgout, S. MacLachlan, T. Manteuffel, S. McCormick and J. Ruge, *"Adaptive Smoothed Aggregation (_SA),"* SIAM Journal of Scientific Computing, **25**, 1896-1920, 2004.

S. W. Bruenn, *"Issues with Core-Collapse Supernova Progenitor Models,"* in Open Issues in Core Collapse Supernova Theory, Proc. of the Institute for Nuclear Theory, Vol. 14, p. 99, University of Washington, Seattle, Wash., June 2004.

N. Bucciantini, R. Bandiera, J. M. Blondin, E. Amato, L. Del Zanna, *"The effects of spin-down on the structure and evolution of pulsar wind nebulae,"* Astronomy & Astrophysics, **422**, 609-619, 2004.

A. Burrows, S. Reddy, and T. A. Thompson, *"Neutrino Opacities in Nuclear Matter,"* Nuclear Physics A, in press, 2004.

J. R. Burruss, et al., *"Remote Computing on the National Fusion Grid,"* The 4th IAEA Technical Meeting on Control, Data Acquisition, and Remote Participation for Fusion Research. Fusion Engineering and Design **71**, 251-255, 2004.

L. Bytautas and K. Ruedenberg, *"Correlation Energy Extrapolation Through Intrinsic Scaling. I,"* Journal of Chemical Physics, **121**, 10905, 2004.

L. Bytautas and K. Ruedenberg, *"Correlation Energy Extrapolation Through Intrinsic Scaling. II,"* Journal of Chemical Physics, **121**, 10919, 2004.

L. Bytautas and K. Ruedenberg, *"Correlation Energy Extrapolation Through Intrinsic Scaling. III. Compact Wavefunctions,"* Journal of Chemical Physics, **121**, 10852, 2004.

A. C. Calder, L. J. Dursi, B. Fryxell, T. Plewa, V. G. Weirs, T. Dupont, H. F. Robey, R. P. Drake, B. A. Remington, G. Dimonte, J. Hayes, J. M. Stone, P. M. Ricker, F. X. Timmes, M. Zingale and K. Olson, *"Issues with Validating an Astrophysical Simulation Code,"* Computing in Science and Engineering, **6**(5):10, 2004.

C. Y. Cardall, A. O. Razoumov, E. Endeve, A. Mezzacappa, *"The Long Term: Six-dimensional Core-collapse Supernova Models,"* in Open Issues in Core Collapse Supernova Theory, Proc. of the Institute for Nuclear Theory, Vol. **14**, p. 196, University of Washington, Seattle, Wash., June 2004.

G. R. Carr, I. L. Carpenter, M. J. Cordery, J. B. Drake, M. W. Ham, F. M. Hoffman and P. H. Worley, *"Porting and Performance of the Community Climate System Model (CCSM3) on the Cray X1,"* Proc. of the 11th Workshop on High Performance Computing in Meteorology, Reading, UK, Oct. 2004.

L. Carrington, N. Wolter, A. Snavely and C. B. Lee, *"Applying an Automated Framework to Produce Accurate Blind Performance Predictions of Full-Scale HPC Applications,"* DOD User Group Conference 2004, Williamsburg, Va., June 2004.

Y. Chen, et al., *"Chiral Logs in Quenched QCD,"* Physical Review D, **70**, 034502, 2004.

Z. Chen, J. Dongarra, P. Luszczek, and K. Roche, *"LAPACK for Clusters Project: An Example of Self Adapting Numerical Software,"* Hawaii International Conference on System Sciences (HICSS-37), Jan. 2004.

S. Chu, M. Maltrud, S. Elliott, J. L. Hernandez and D. J. Erickson III, *"Ecodynamic and eddy resolving dimethyl sulfide simulations in a global ocean biogeochemistry/circulation model,"* Earth Interactions, **8** (11), 1, 2004.

S. Chu, S. Elliott, M. E. Maltrud, F. Chavez and F. Chai, *"Ecodynamics of multiple Southern Ocean iron enrichments simulated in a global, eddy permitting GCM,"* in Environmental Sciences and Environmental Computing Vol. II, The EnviroComp Institute, 2004.

S. Chu, S. Elliott, M. E. Maltrud, F. Chavez, and F. Chai, *"Southern Ocean Iron Enrichments Simulated in a global, eddy permitting GCM,"* in Environmental Sciences and Environmental Computing Vol. II, ed. P. Zannetti, The EnviroComp Institute, 2004.

I.-H. Chung, and J. K. Hollingsworth, *"Using Information from Prior Runs to Improve Automated Tuning Systems,"* Proc. of ACM/IEEE SC2004 conference, Pittsburgh, Penn., Nov. 2004.

I.-H. Chung, and J. K. Hollingsworth, *"Automated Cluster-Based Web Service Performance Tuning,"* Proceedings of IEEE Conference on High Performance Distributed Computing (HPDC), June 2004.

J. P. Colgan, M. S. Pindzola, and N. R. Badnell, *"Dielectronic recombination data for dynamic finite-density plasmas: V. The Lithium isoelectronic sequence,"* Astronomy and Astrophysics, **417**, 1183, 2004.

J. P. Colgan and M. S. Pindzola, *"Double photoionization of helium at high photon energies,"* Journal of Physics B, **37**, 1153, 2004.

D. Crawford, K.-L. Ma, M.-Y. Huang, S. Klasky and S. Ethier, *"Visualizing Gyrokinetic Simulations,"* Proc. of the IEEE Visualization 2004 conference, Austin, Texas, Oct. 2004.

T. L. Dahlgren, P. T. Devanbu, *"Adaptable Assertion Checking for Scientific Software Components,"* Proc. of the First International Workshop on Software Engineering for High Performance Computing System Applications, Edinburgh, Scotland, UK, p 64-69, May 2004.

D. Datta, R. C. Picu, M. S. Shephard, *"Composite Grid Atomistic Continuum Method: An adaptive approach to bridge continuum with atomistic analysis,"* Journal of Multiscale Computational Engineering, **2**(3), p. 401-420, 2004.

C. T. H. Davies, et al., *"High-Precision Lattice QCD Confronts Experiment,"* Physical Review Letters, **92**, 022001, 2004.

T. A. Davis, J. R. Gilbert, S. I. Larimore, and E. G. Ng, *"A column approximate minimum degree ordering algorithm,"* ACM Transactions of Mathematical Software **30**, p. 353-376, 2004.

T. A. Davis, J. R. Gilbert, S. I. Larimore, and E. G. Ng, *"Algorithm 836: COLAMD, a column approximate minimum degree ordering algorithm,"* ACM Transactions of Mathematical Software **30**, p. 377-380, 2004.

D. J. Dean, *"Intersections of Nuclear Physics and Astrophysics,"* in The Future Astronuclear Physics, A. Jorissen, S. Goriely, M. Rayet, L. Siers, J. Boffin, eds., EAS Publications Series, p. 175-189, 2004.

H. de Sterck, T. Manteuffel, S. McCormick, and L. Olson, *"Least-squares finite element methods and algebraic multigrid solvers for linear hyperbolic PDEs,"* SIAM Journal of Scientific Computing, **26**, 31-54, 2004.

S. Deng et al., *"Plasma wakefield acceleration in self-ionized gas or plasmas,"* Physical Review E **68**, 047401, 2004.

Y. Deng, J. Glimm, J. Davenport, X. Cai, E. Santos, *"Performance models on QCDOC for molecular dynamics with coulomb potentials,"* International Journal of High Performance Computing Applications, **18**, p. 183-198, 2004.

M. di Pierro et al., *"Properties of charmonium in lattice QCD with 2+1 flavors of improved staggered sea quarks,"* Nuclear Physics (Proc. Suppl.) 129-130, 340. 2004.

M. di Pierro, et al., *"Ds spectrum and leptonic decays with Fermilab heavy quarks and improved staggered light quarks,"* Nuclear Physics (Proc. Suppl.) 129-130, 328, 2004.

J. B. Drake, P. H. Worley, I. Carpenter, M. Cordery, *"Experience with the Full CCSM,"* Proc. of the 46th Cray User Group Conference, Knoxville, TN, May 2004.

M. Dryja, A. Gantner, O. Widlund, and B. I. Wohlmuth, *"Multilevel Additive Schwarz Preconditioner for Nonconforming Mortar Finite Element Methods,"* Journal on Numerical Analysis, Math., **12**, 1, 23-38, 2004.

T. H. Dunigan, Jr., J. S. Vetter, and P. H. Worley, *"Performance Evaluation of the Cray X1 Distributed Shared Memory Architecture,"* Proc. of IEEE Hot Interconnects, 2004.

S. Dutta, J. Glimm, J. W. Grove, D. H. Sharp, Y. Zhang, *"Error comparison in tracked and untracked spherical simulations,"* Computers and Mathematics with Applications, **48**, p. 1733-1747, 2004.

S. Dutta, J. Glimm, J. W. Grove, D. H. Sharp, Y. Zhang, *"Spherical Richtmyer-Meshkov instability for axisymmetric flow,"* Mathematics and Computers in Simulations, **65**, p. 417-430, 2004.

S. I. Dutta, S. Ratkovic, M. Prakash, *"Photoneutrino process in astrophysical systems,"* Physical Review D, **69**, 023005, 2004.

R. G. Edwards, G. Fleming, D. G. Richards, H. R. Fiebig and The LHPC Collaboration, *"Lattice QCD and nucleon resonances,"* Nuclear Physics A, **737**, 167, 2004.

S. Elliott, S. Chu, M. Maltrud and A. McPherson, *"Animation of global marine chlorophyll distributions from fine grid biogeochemistry/transport modeling,"* in Environmental Sciences and Environmental Computing Vol. II (Edited by P. Zannetti), The EnviroComp Institute, 2004.

S. Ethier and Z. Lin, *"Porting the 3D gyrokinetic particle-in-cell code GTC to the NEC SX-6 vector architecture: perspectives and challenges,"* Computer Physics Communications, **164**, 456, 2004.

R. D. Falgout and P. S. Vassilevski, *"On Generalizing the AMG Framework,"* SIAM Journal on Numerical Analysis, **42**, p. 1669-1693, 2004.

D. G. Fedorov, R. M. Olson, K. Kitaura, M. S. Gordon, and S. Koseki, *"A new hierarchical parallelization scheme: Generalized distributed data interface (GDDI), and an application to the fragment molecular orbital method (FMO),"* Journal of Computational Chemistry, **25**, 872, 2004.

S. Flanagan, et al., *"A General Purpose Data Analysis Monitoring System with Case Studies from the National Fusion Grid and the DIII-D MDSplus between Pulse Analysis System,"* 4th IAEA Technical Meeting on Control, Data Acquisition, and Remote Participation for Fusion Research, Fusion Engineering and Design **71**, 263-267, 2004.

E. Follana, et al. (The HPQCD Collaboration), *"Improvement and taste symmetry breaking for staggered quarks,"* Nuclear Physics (Proc. Suppl.) 129-130, 384, 2004.

N. Folwell, L. Ge, A. Guetz, V. Ivanov, et al., *"Electromagnetic System Simulation – Prototyping Through Computation,"* SciDAC PI meeting, 2004.

C. L. Fryer, *"Neutron Star Kicks from Asymmetric Collapse,"* ApJ Letters, **601**:L175-L178, Feb. 2004.

C. L. Fryer, D. E. Holz, and S. A. Hughes, *"Gravitational Waves from Stellar Collapse: Correlations to Explosion Asymmetries,"* ApJ, **609**:288-300, July 2004.

C. L. Fryer and M. S. Warren, *"The Collapse of Rotating Massive Stars in Three Dimensions,"* American Physics Journal, **601**:391-404, Jan. 2004.

L. Ge, L.-Q. Lee, Z. Li, C.-K. Ng, K. Ko, Y. Luo and M. Shephard, *"Adaptive Mesh Refinement For High Accuracy Wall Loss Determination In Accelerating Cavity Design,"* Proc. of the Eleventh Biennial IEEE Conference on Electromagnetic Field Computation, Seoul, Korea, June 2004.

L. Ge, L. Lee, L. Zenghai, L. Ng, C. Ko, K., Y. Luo, M. S. Shephard, *"Adaptive Mesh Refinement for High Accuracy Wall Loss Determination in Accelerating Cavity Design,"* IEEE Conf. on Electromagnetic Field Computations, June 2004.

C. G. R. Geddes, C. Toth, J. van Tilborg, E. Esarey, C. B. Schroeder, D. Bruhwiler, C. Nieter, J. Cary and W. P. Leemans, *"High-quality electron beams from a laser wakefield accelerator using plasma-channel guiding,"* Nature **431**, p.538-541, 2004.

J. Glimm, J. W. Grove, Y. Kang, T. Lee, X. Li, D. H. Sharp, Y. Yu, K. Ye, M. Zhao, *"Statistical riemann problems and a composition law for errors in numerical solutions of shock physics problems,"* SIAM Journal on Scientific Computing, **26**, p. 666-697, 2004.

J. Glimm, S. Hou, Y. Lee, D. Sharp, K. Ye, *"Sources of uncertainty and error in the simulation of flow in porous media,"* Comp. and Applied Mathematics, **23**, p. 109-120, 2004.

J. Glimm, H. Jin, Y. Zhang, *"Front tracking for multiphase fluid mixing,"* Computational Methods in Multiphase Flow II, A. A. Mammoli, C. A. Brebbia, eds., p. 13-22, WIT Press, Southampton, UK, 2004.

J. N. Goswami, K. K. Marhas, M. Chaussidon, M. Gounelle, B. Meyer, *"Origin of Short-lived Radionuclides in the Early Solar System,"* Workshop on Chondrites and the Protoplanetary Disk, p. 9120, 2004.

J. F. Grcar, P. Glarborg, J. B. Bell, M. S. Day, A. Loren, and A. D. Jenson, *"Effects of Mixing on Ammonia Oxidation in Combustion Environments at Intermediate Temperatures,"* Proceedings of the Combustion Institute, **30**:1193, 2004.

L. Grigori and X. S. Li, *"Performance Analysis of Parallel Right-looking Sparse LU Factorization on Two-dimensional Grids of Processors,"* Proceedings of the PARA'04 Workshop on State-of-the art in Scientific Computing, Springer Lecture Notes in Computer Science, 2004.

Y. Guo, A. Kawano, D. L. Thompson, A. F. Wagner and M. Minkoff, *"Interpolating Moving Least-Squares Methods for Fitting Potential Energy Surfaces: Applications to Classical Dynamics Calculations,"* Journal of Chemical Physics, **121**, 5091-5097, 2004.

A. Gurtler, F. Robicheaux, W. J. van der Zande and L. D. Noordam, *"Asymmetry in the strong field ionization of Rydberg atoms by few-cycle pulses,"* Physical Review Letters, 033002, 2004.

A. Gurtler, F. Robicheaux, M. J. J. Vrakking, W. J. van der Zande and L. D. Noordam, *"Carrier phase dependence in the ionization of Rydberg atoms by short radio-frequency pulses: a model system for high order harmonic generation,"* Physical Review Letters, **92**, 063901, 2004.

S. W. Hadley, D. J. Erickson III, J. L. Hernandez and S. Thompson, *"Future U.S. energy use for 2000-2025 as computed with temperatures from a global climate prediction model and energy demand model,"* Proc. of the 24th Annual North American Conference of the USAEE/IAEE, United States Association for Energy Economics, Cleveland, OH, 2004.

P. T. Haertel, D. A. Randall and T. G. Jensen, *"Toward a Lagrangian ocean model: Simulating upwelling in a large lake using slippery sacks,"* Monthly Weather Review, **132**, 66, 2004.

A. T. Hagler, et al. (The LHPC Collaboration), *"Transverse structure of nucleon parton distributions from lattice QCD,"* Physical Review Letters, **93**, 112001, 2004.

W. C. Haxton, *"Supernova Neutrino-Nucleus Physics and the r-Process,"* The r-Process: The Astrophysical Origin of the Heavy Elements and Related Rare Isotope Accelerator Physics, Proc. of the First Argonne/MSU/JINA/INT R/A Workshop, p. 73, World Scientific, 2004.

Y. He and C. Ding, *"MPI and OpenMP Paradigms on Cluster of SMP Architectures: the Vacancy Tracking Algorithm for Multi-Dimensional Array Transpose,"* Journal of Parallel and Distributed Computing Practice, **2**, 5, 2004.

E. D. Held, J. D. Callen, C. C. Hegna, C. R. Sovinec, T. A. Gianakon, S. E. Kruger, *"Nonlocal closures for plasma fluid simulations,"* Physics of Plasmas **11**, 2419, 2004.

J. J. Heys, C. G. DeGroff, T. Manteuffel, S. McCormick, and H. Tufo, *"Modeling 3-d compliant blood flow with FOSLS,"* Biomed Sci Instrum. **40**, p. 193-9, 2004.

J. Heys, T. Manteuffel, S. McCormick, and L. Olson, *"Algebraic multigrid (AMG) for higher-order finite elements,"* Journal of Computational Physics **195**, p. 560-575, 2004.

J. Heys, T. Manteuffel, S. McCormick, and J. Ruge, *"First-order system least squares (FOSLS) for coupled fluid-elasticity problems,"* Journal of Computational Physics **195**, p. 560-575, 2004.

D. Higdon, M. Kennedy, J. C. Cavendish, J. A. Cafeo, R. D. Ryne, *"Combining Field Data and Computer Simulations for Calibration and Prediction,"* SIAM Journal on Scientific Computing, **26**, 2, p. 448-466, March 2004.

W. R. Hix, O. E. B. Messer, A. Mezzacappa, *"The interplay between nuclear electron capture and fluid dynamics in core collapse supernovae,"* in Cosmic explosions in Three Dimensions, P. Hoflich, P. Kumar, J. C. Wheeler, eds., p. 307, Cambridge University Press, 2004.

F. M. Hoffman, M. Vertenstein, H. Kitabata, J. B. White III, P. H. Worley, J. B. Drake, M. Cordery, *"Adventures in Vectorizing the Community Land Model,"* Proc. of the 46th Cray User Group Conference, Knoxville, TN, May 2004.

I. Hofmann, G. Franchetti, J. Qiang, R. D. Ryne, *"Dynamical Effects of the Montague Resonance,"* Proc. EPAC 2004, Lucerne, Switzerland, p. 1960, 2004.

I. Hofmann, G. Franchetti, M. Giovannozzi, M. Martini, E. Metral, J. Qiang, R. D. Ryne, *"Simulation aspects of the code benchmarking based on the CERN-PS Montague-resonance experiment,"* Proc. 33rd ICFA Advanced Beam Dynamics Workshop on High Intensity & High Brightness Hadron Beams, Bensheim, Germany, Oct. 2004.

D. J. Holmgren, P. Mackenzie, A. Singh and J. Somine, *"Lattice QCD clusters at Fermilab,"* Computing in High-Energy Physics (CHEP '04), Interlaken, Switzerland, Sept. 2004.

U. Hwang, J. M. Laming, C. Badenes, F. Berendse, J. Blondin, D. Cio, T. DeLaney, D. Dewey, R. Fesen, K. A. Flanagan, C. L. Fryer, P. Ghavamian, J. P. Hughes, J. A. Morse, P. P. Plucinsky, R. Petre, M. Pohl, L. Rudnick, R. Sankrit, P. O. Slane, R. K. Smith, J. Vink, and J. S. Warren, *"A Million*

Second Chandra View of Cassiopeia A.," ApJ Letters, 615, L117-L120, Nov. 2004.

A. V. Ilin, F. R. Chang-Diaz, J. P. Squire, A. G. Tarditi, M. D. Carter, *"Improved simulation of the ICRF waves in the VASIMR plasma,"* Proceedings of the 18th International conference on the numerical Simulation of Plasmas, Computer Physics Communications **164**, 251, 2004.

E.-J. Im, I. Bustany, C. Ashcraft, J. Demmel and K. Yelick, *"Toward automatic performance tuning of matrix triple products based on matrix structure,"* PARA'04 Workshop on State-of-the-art in Scientific Computing, Copenhagen, Denmark, June 2004.

E.-J. Im, K. A. Yelick and R. Vuduc, *"SPARSITY: An Optimization Framework for Sparse Matrix Kernels,"* International Journal of High Performance Computing Applications, **18** (1), p. 135-158, Feb. 2004.

J. P. Iorio, P. B. Duffy, B. Govindasamy, S. L. Thompson, M. Khairoutdinov and D. A. Randall, *"Effects of model resolution and subgrid-scale physics on the simulation of daily precipitation in the continental United States,"* Climate Dynamics, **23**, 243, 2004.

L. Ives, T. Bui, W. Vogler, A. Bauer, M. Shephard, *"Operation and performance of a 3D finite element charged particle code with adaptive meshing Source,"* 5th IEEE Int. Vacuum Electronics Conf. (IVEC 2004), p. 316-317, 2004.

C. Jablonowski, *"Adaptive grids in weather and climate modeling,"* University of Michigan thesis, 2004.

C. Jablonowski, M. Herzog, J. E. Penner, R. Oehmke, Q. F. Stout, B. van Leer, *"Adaptive grids for weather and climate models,"* ECMWF Seminar Proceedings on Recent Developments in Numerical Methods for Atmospheric and Ocean Modelling, Reading, UK, Sept. 2004.

S. C. Jardin, *"A triangular finite element with first-derivative continuity applied to fusion MHD applications,"* Journal of Computational Physics **200**, 133, 2004.

G. C. Jordan, B. S. Meyer, *"Nucleosynthesis in Fast Expansions of High-Entropy, Proton-rich Matter,"* Astrophysical Journal Letters, **617**, L131-L134, 2004.

G. C. Jordan, B. S. Meyer, *"Nuclear Reaction Rates and the Production of Light p-Process Isotopes in Fast Expansions of Proton-Rich Matter,"* The r-Process: The Astrophysical Origin of the Heavy Elements and Related Rare Isotope Accelerator Physics, Proc. of the First Argonne/MSU/JINA/INT R/A Workshop, p. 157, World Scientific, 2004.

R. Katz, M. Knepley and B. Smith, *"Developing a Geodynamics Simulation with PETSc,"* in Numerical Solution of Partial Differential Equations on Parallel Computers, A. M. Bruaset, P. Bjorstad, and A. Tveito, eds., p. 413, Springer-Verlag, 2004.

S. R. Kawa, D. J. Erickson III, S. Pawson, and Z. Zhu, *"Global CO2 transport simulations using meteorological data from the NASA data assimilation system,"* Journal of Geophysical Research, **109**. D18, 2004.

K. Keahey et al., *"Agreement Based Interactions for Experimental Science,"* Proc. of Europar 2004 conference, 2004.

K. Keahey, et al., *"Grids for Experimental Science: The Virtual Control Room,"* Proc. of the CLADE 2004 Workshop, 2004.

K. Keahey, et al., *"Fine-Grained Authorization for Job Execution in the Grid: Design and Implementation,"* Concurrency and Computation: Practice and Experience **16** (5), 477-488, 2004.

J. P. Kenny, S. J. Benson, Y. Alexeev, J. Sarich, C. L. Janssen, L. Curfman McInnes, M. Krishnan, J. Nieplocha, E. Jurrus, C. Fahlstrom and T. L. Windus, *"Component-Based Integration of Chemistry and Optimization Software,"* Journal of Computational Chemistry, **25**, 1717-1725, 2004.

M. E. Kowalski, C.-K. Ng, L.-Q. Lee, Z. Li and K. Ko, *"Time-Domain Calculation of Guided Electromagnetic Wave Propagation on Unstructured Grids,"* U. S. National Committee of the International Union of Radio Science (URSI) National Radio Science Meeting, Boulder, Colo., Jan. 2004.

B. C. Lee, R. Vuduc, J. Demmel and K. Yelick, *"Performance Models for Evaluation and Automatic Tuning of Symmetric Sparse Matrix-Vector Multiply,"* International Conference on Parallel Processing, Montreal, Quebec, Canada, Aug. 2004.

L.-Q. Lee, L. Ge, M. Kowalski, Z. Li, C.-K. Ng, G. Schussman, M. Wolf and K. Ko, *"Solving Large Sparse Linear Systems In End-To-End Accelerator Structure Simulations,"* Proc. of the 18th International Parallel and Distributed Processing Symposium, Santa Fe, NM, April 2004.

T. Lee, Y. Yu, M. Zhao, J. Glimm, X. Li, K. Ye, *"Error analysis of composite shock interaction problems,"* Proc. of PMC04 Conference, 2004.

W. W. Lee, *"Theoretical and numerical properties of a gyrokinetic plasma: implications on transport scale simulation,"* Computer Physics Communications, **164**, 244, 2004.

W. W. Lee, *"Steady State Global Simulations of Microturbulence,"* American Physical Society Division of Plasma Physics, Savannah, Ga., Nov. 2004.

J. Li and O. Widlund, *"FETI--DP, BDDC, and Block Cholesky Methods,"* International Journal on Numerical Analysis, Methods Engineering, 2004.

N. Li, Y. Saad and E. Chow, *"Crout Versions of ILU for General Sparse Matrices,"* SIAM Journal of Scientific Computing, **25**, p. 716-728, 2004.

X. Li, J. F. Remacle, N. Chevaugeon, M. S. Shephard, *"Anisotropic Mesh Gradation Control,"* 13th International Meshing Roundtable, Sandia National Laboratories, p. 401-412, 2004.

Z. Li, N. T. Folwell, L. Ge, A. Guetz, V. Ivanov, M. Kowalski, L.-Q. Lee, C.-K. Ng, G. Schussman, R. Uplenchwar, M. Wolf and K. Ko, *"X-Band Linear Collider R&D In Accelerating Structures Through Advanced Computing,"* Proc. of the 9th European Particle Accelerator Conference, Lucerne, Switzerland, July 2004.

Z. Li, N. Folwell, L. Ge, A. Guetz, V. Ivanov, M. Kowalski, L.-Q. Lee, C.-K. Ng, G. Schussman, R. Uplenchwar, M. Wolf, L. Xiao and K. Ko, *"High Performance Computing In Accelerator Structure Design And Analysis,"* Proc. of the 8th International Computational Accelerator Physics Conference, St. Petersburg, Russia, June 2004.

M. Liebendoerfer, O. E. B. Messer, A. Mezzacappa, S. W. Bruenn, C. Y. Cardall, F.-K. Thielemann, *"A Finite Difference Representation of Neutrino Radiation Hydrodynamics in Spherically Symmetric General Relativistic Spacetime,"* Astrophysical Journal Supplement Series, **150**, 263-316, 2004.

Y. Lin, S. Wukitch. P. Bonoli, E. Nelson-Melby, M. Porkolab, J. C. Wright, N. Basse, A. E. Hubbard, J. Irby, L. Lin, E. S.

Marmar, A. Mazurenko, D. Mossessian, A. Parisot, J. Rice, S. Wolfe, C. K. Phillips, G. Schilling, J. R. Wilson, P. Phillips and A. Lynn, *"Investigation of Ion Cyclotron Range of Frequencies Mode Conversion at the Ion-Ion Hybrid Layer in Alcator C-Mod,"* Physics of Plasmas **11** (5) 2466-2472, 2004.

Z. Lin and T. S. Hahm, *"Turbulence spreading and transport scaling in global gyrokinetic particle simulations,"* Physics of Plasmas, **11**, 1099, 2004.

Z. Lin et al., *"Electron Thermal Transport in Tokamaks: ETG or TEM Turbulence?"* International Atomic Energy Agency Conference, IAEA-CN/TH/8-4, Vilamoura, Portugal, 2004.

W. Lipscomb and T. D. Ringler, *"An incremental remapping transport scheme on a spherical geodesic grid,"* Monthly Weather Review, **133**, 2335, 2004.

E. Livne, A. Burrows, R. Walder, I. Lichtenstadt and T. A. Thompson, *"Two-dimensional, Time-dependent, Multigroup, Multiangle Radiation Hydrodynamics Test Simulation in the Core-Collapse Supernova Context,"* Astrophysical Journal, **609**:277-287, July 2004.

S. D. Loch, C. J. Fontes, J. P. Colgan, M. S. Pindzola, C. P. Ballance, D. C. Griffin, M. G. O'Mullane and H. P. Summers, *"A collisional-radiative study of lithium plasmas,"* Physical Review E, **69**, 066405, 2004.

C. Lu and D. Reed, *"Assessing Fault Sensitivity in MPI Applications,"* Proc. of the ACM/IEEE SC2004 conference, Pittsburgh, Penn., Nov. 2004.

X. J. Luo, M. S. Shephard, R. M. O'Bara, R. Nastasia, M. W. Beall, *"Automatic p-version mesh generation for curved domains,"* Book of Abstracts: ICOSAHOM 4004, Brown University, June, 2004.

X. J. Luo, M. S. Shephard, R. M. O'Bara, R. Nastasia, M. W. Beall., *"Automatic p-version mesh generation for curved domains,"* Engineering with Computers, **20**(3), p. 273-285, 2004.

K.-L. Ma and E. Lum, *"Techniques for Visualizing Time-Varying Volume Data,"* in Visualization Handbook, C. Hansen and C. Johnston, eds., Academic Press, Oct. 2004.

K.-L. Ma, G. Schussman and B. Wilson, *"Visualization for Computational Accelerator Physics,"* in Visualization Handbook, C. Hansen and C. Johnston, eds., Academic Press, Oct. 2004.

H. MacMillan, T. Manteuffel and S. McCormick, *"First-order system least squares and electrical impedance tomography,"* SIAM Journal on Numerical Analysis, **42**, p. 461-483, 2004.

G. Mahinthakumar, M. Sayeed, J. Blondin, P. Worley, W. Hix and A. Mezzacappa, *"Performance Evaluation and Modeling of a Parallel Astrophysics Application,"* Proc. of the High Performance Computing Symposium 2004, The Society for Modeling and Simulation International, Arlington, Va., 2004.

G. G. Maisuradze, A. Kawano, D. L. Thompson, A. F. Wagner, and M. Minkoff, *"Interpolating Moving Least-Squares Methods for Fitting Potential Energy Surfaces: Analysis of an Application to a Six-Dimensional System,"* Journal of Chemical Physics, **121**, 10329-10338, 2004.

G. Martinez-Pinedo, K. Langanke, J. M. Sampaio, D. J. Dean, W. R. Hix, O. E. B. Messer, A. Mezzacappa, M. Liebendorfer, H.-T. Janka, M. Rampp, *"Weak Interaction Processes in Core-Collapse Supernovae,"* IAU Colloq. 192: Cosmic Explosions, On the 10th Anniversary of SN1993J, p. 321, 2005.

N. Mathur, et al., *"A Study of Pentaquarks on the Lattice with Overlap Fermions,"* Physical Review D, **70**, 074508, 2004.

B. S. Lee McCormick, B. Philip, and D. Quinlan, *"Asynchronous fast adaptive composite-grid methods for elliptic problems: theoretical foundations,"* SIAM Journal on Numerical Analysis, **42**, p. 130-152, 2004.

P. McCorquodale, P. Colella, D. P. Grote, J.-L. Vay, *"A node-centered local refinement algorithm for Poisson's equation in complex geometries,"* Journal of Computational Physics, **201**, p. 34-60, 2004.

E. Métral, C. Carli, M. Giovannozzi, M. Martini, R. R. Steerenberg, G. Franchetti, I. Hofmann, J. Qiang, R. D. Ryne, *"Intensity Dependent Emittance Transfer Studies at the CERN Proton Synchrotron,"* Proc. EPAC 2004, Lucerne, Switzerland, p. 1894, 2004.

E. Métral, M. Giovannozzi, M. Martini, R. R. Steerenberg, G. Franchetti, I. Hofmann, J. Qiang, R. D. Ryne, *"Space-Charge Experiments at the CERN Proton Synchrotron,"* Proc. 33rd ICFA Advanced Beam Dynamics Workshop on High Intensity & High Brightness Hadron Beams, Bensheim, Germany, Oct., 2004.

B. S. Meyer, *"Synthesis of Short-lived Radioactivities in a Massive Star,"* ASP Conf. Ser. 341: Chondrites and the Protoplanetary Disk, p. 515, 2005.

B. S. Meyer, *"Online Tools for Astronomy and Cosmochemistry,"* 36th Annual Lunar and Planetary Science Conference, p. 1457, 2005.

B. S. Meyer, *"Nucleosynthesis of Short-lived Radioactivities in Massive Stars,"* Workshop on Chondrites and the Protoplanetary Disk, p. 9089, 2004.

P. A. Milne, A. L. Hungerford, C. L. Fryer, T. M. Evans, T. J. Urbatsch, S. E. Boggs, J. Isern, E. Bravo, A. Hirschmann, S. Kumagai, P. A. Pinto, and L.-S. The, *"Unified One-Dimensional Simulations of Gamma-Ray Line Emission from Type Ia Supernovae,"* Astrophysical Journal, **613**:1101-1119, Oct. 2004.

P. Mucci, J. Dongarra, R. Kufrin, S. Moore, F. Song, F. Wolf, "*Automating the Large-Scale Collection and Analysis of Performance,"* Proc. of the 5th LCI International Conference on Linux Clusters: The HPC Revolution, Austin, Texas, May 2004.

P. Muggli, B. E. Blue, C. E. Clayton, S. Deng, F.-J. Decker, M. J. Hogan, C. Huang, R. Iverson, C. Joshi, T. C. Katsouleas, S. Lee, W. Lu, K. A. Marsh, W. B. Mori, C. L. O'Connell, P. Raimondi, R. Siemann, and D. Walz, *"Meter-Scale Plasma-Wakefield Accelerator Driven by a Matched Electron Beam,"* Physical Review Special Topics-Accelerators and Beams **93**, 014802, 2004.

J. W. Murphy, A. Burrows and A. Heger, *"Pulsational Analysis of the Cores of Massive Stars and Its Relevance to Pulsar Kicks,"* Astrophysical Journal, **615**:460-474, Nov. 2004.

J. D. Myers, T. C. Allison, S. Bittner, D. Didier, M. Frenklach, W. H. Green, Jr., Y.-L. Ho, J. Hewson, W. Koegler, C. Lansing, D. Leahy, M. Lee, R. McCoy, M. Minkoff, S. Nijsure, G. von Laszewski, D. Montoya, L. Oluwole, C. Pancerella, R. Pinzon, W. Pitz, L. A. Rahn, B. Ruscic, K. Schuchardt, E. Stephan, A. Wagner, T. Windus, C. Yang, *"A collaborative informatics infrastructure for multi-scale science,"* Challenges of Large Applications in Distributed Environments (CLADE) Workshop, Honolulu, Hawaii, June 2004.

J. R. Myra, L. A. Berry, D. A. D'Ippolito, E. F. Jaeger, *"Nonlinear Fluxes and Forces from Radio-Frequency Waves with Application to Driven Flows in Tokamaks,"* Physics of Plasmas **11**, 1786, 2004.

D. Narayan, R. Bradshaw, A. Lusk and E. Lusk, *"MPI cluster system software,"* Recent Advances in Parallel Virtual Machine and Message Passing Interface, Lecture Notes in Computer Science, **3241**, p. 277-286. Springer-Verlag, 2004.

D. Narayan, R. Bradshaw, A. Lusk, E. Lusk and R. Butler, *"Component-based cluster systems software architecture: A case study,"* Proc. of the 6th IEEE International Conference on Cluster Computing (CLUSTER04), p. 319-326, IEEE Computer Society, 2004.

J. W. Negele, et al. (The LHPC Collaboration), *"Insight into nucleon structure from generalized parton distributions,"* Nuclear Physics (Proc. Suppl.) 129-130, 910, 2004.

J. W. Negele, et al., *"Insight into nucleon structure from lattice calculations of moments of parton and generalized parton distributions,"* Nuclear Physics (Proc. Suppl.) **128**, 170, 2004.

J. W. Negele, *"What we are learning about the quark structure of hadrons from lattice QCD,"* 3rd International Symposium on the Gerasimov-Drell-Hearn Sum Rule and its Extensions (GDH 2004), Norfolk, Virginia, June 2004.

C.-K. Ng, N. Folwell, A. Guetz, V. Ivanov, L.-Q. Lee, Z. Li, G. Schussman and K. Ko, *"Simulating Dark Current In Nlc Structures,"* Proc. of the 8th International Computational Accelerator Physics Conference, St. Petersburg, Russia, June 2004.

M. A. Nobes and H. D. Trottier, *"Progress in automated perturbation theory for heavy quark physics,"* Nuclear Physics (Proc. Suppl.) 129-130, 355, 2004.

B. Norris, J. Ray, R. C. Armstrong, L. C. McInnes, D. E. Bernholdt, W. R. Elwasif, A. D. Malony and S. Shende, *"Computational quality of service for scientific components,"* Proc. of the International Symposium on Component-Based Software Engineering (CBSE7), Edinburgh, Scotland, May 2004.

K. Ohmi, M. Tawada, Y. Cai, S. Kamada, K. Oide, J. Qiang, *"Beam-beam limit in e+e- circular colliders,"* Physical Review Letters **92**, 214801, 2004.

K. Ohmi, M. Tawada, Y. Cai, S. Kamada, K. Oide, and J. Qiang, *"Luminosity limit due to the beam-beam interactions with or without crossing angle,"* Physical Review ST Accel. Beams, vol **7**, 104401, 2004.

C. D. Ott, A. Burrows, E. Livne and R. Walder, *"Gravitational Waves from Axisymmetric, Rotating Stellar Core Collapse,"* Astrophysical Journal, **600**:834-864, Jan. 2004.

S. Ovtchinnikov and X.-C. Cai, *"One-level Newton-Krylov-Schwarz algorithm for unsteady nonlinear radiation diffusion problem,"* Numerical Linear Alg. Applic., **11**, 867-881, 2004.

P. P. Pebay, H. N. Najm, and J. Pousin, *"A Non-Split Projection Strategy for Low Mach Number Reacting Flow,"* International Journal of Multiscale Computational Eng., **2**(3):445-460, Aug. 2004.

P. Petreczky and K. Petrov, *"Free energy of a static quark anti-quark pair and the renormalized Polyakov loop in three flavor QCD,"* Physical Review D, **70**, 054503, 2004.

M. Prakash, et al., *"Neutrino Processes in Supernovae and Neutron Stars in Their Infancy and Old Age,"* in Compact Stars: The Quest for New States of Dense Matter, Proc. of the KIAS-APTCP International Symposium on Astro-Hadron Physics, Seoul, Korea, p. 476, 2004.

J. Pruet, R. Surman and G. C. McLaughlin, *"On the Contribution of Gamma-Ray Bursts to the Galactic Inventory of Some Intermediate-Mass Nuclei,"* Astrophysical Journal Letters, **602**:L101-L104, Feb. 2004.

J. Pruet, T. A. Thompson and R. D. Hoffman, *"Nucleosynthesis in Outflows from the Inner Regions of Collapsars,"* Astrophysical Journal, **606**:1006-1018, May 2004.

J. Qiang, M. Furman and R. Ryne, *"A Parallel Particle-In-Cell Model for Beam-Beam Interactions in High Energy Ring Colliders,"* Journal of Computational Physics vol. **198**, 278, 2004.

J. Qiang and R. Gluckstern, *"Three-Dimensional Poisson Solver for a Charged Beam with Large Aspect Ratio in a Conducting Pipe,"* Computer Physics Communications, **160**, 120, 2004.

J. Qiang, R. D. Ryne, I. Hofmann, *"Space-charge driven emittance growth in a 3D mismatched anisotropic beam,"* Physical Review Letters, **92**, 174801, 2004.

J. Qiang, *"Halo formation due to beam-beam interactions of beams optically mismatched at injection,"* Physical Review ST Accel. Beams, vol **7**, 031001, 2004.

J. Qiang, *"Strong-strong beam-beam simulation on parallel computer,"* ICFA Beam Dynamics Newsletter, No. **34**, p.19-26, 2004.

D. Quinlan, M. Schordan, Q. Yi and A. Saebjornsen, *"Classification and Utilization of Abstractions for Optimization,"* First International Symposium on Leveraging Applications of Formal Methods, Paphos, Cyprus, Oct. 2004.

D. A. Randall, *"The new CSU dynamical core," Seminar on Recent Developments in Numerical Methods of Atmosphere and Ocean Modeling,"* European Centre for Mid-Range Weather Forecasting, UK, Sept. 2004.

D. A. Randall and W. H. Schubert, *"Dreams of a stratocumulus sleeper,"* Atmospheric Turbulence and Mesoscale Meteorology, E. Fedorovich, R. Rotuno and G. Stevens, eds., p. 71, Cambridge University Press, 2004.

K. Robinson, L. J. Dursi, P. M. Ricker, R. Rosner, A. C. Calder, M. Zingale, J. W. Truran, T. Linde, A. Caceres, B. Fryxell, K. Olson, K. Riley, A. Siegel and N. Vladimirova, *"Morphology of Rising Hydrodynamic and Magnetohydrodynamic Bubbles from Numerical Simulations,"* Astrophysical Journal, **601**:621-643, Feb. 2004.

A. L. Rosenberg, J. E. Menard, J. R. Wilson, S. Medley, R. Andre, D. Darrow, R. Dumont, B. P. LeBlanc, C. K. Phillips, M. Redi, T. K. Mau, E. F. Jaeger, P. M. Ryan, D. W. Swain, R. W. Harvey, J. Egedal and the NSTX Team, *"Fast Ion Absorption of the High Harmonic Fast Wave in the National Spherical Torus Experiment,"* Physics of Plasmas **11**, 2441, 2004.

B. Ruscic, *"Active Thermochemical Table,"* in 2005 Yearbook of Science and Technology, an annual update to the McGraw-Hill Encyclopedia of Science and Technology, McGraw-Hill, New York, 2004.

B. Ruscic, R. E. Pinzon, M. L. Morton, G. von Laszewski, S. Bittner, S. G. Nijsure, K. A. Amin, M. Minkoff, A. F. Wagner. 2004, *"Introduction to active thermochemical tables: Several "key" enthalpies of formation revisited,"* Journal of Physical Chemistry A, **108**:9979-9997, 2004.

R. S. Samtaney, S. Jardin, P. Colella, D. F. Martin, *"3D adaptive mesh refinement simulations of pellet injection in tokamaks,"* Computer Physics Communications **164** 1-3 220, 2004.

A. R. Sanderson, et al., *"Display of Vector Fields Using a Reaction-Diffusion Model,"* Proc. of the 2004 IEEE Visualization Conference, 115-122, 2004.

D. P. Schissel, *"The National Fusion Collaboratory Project,"* Proc. of the 2004 DOE SciDAC PI Meeting, 2004.

D. P. Schissel, *"The National Fusion Collaboratory Project: Applying Grid Technology for Magnetic Fusion Research,"* Proc. of the Workshop on Case Studies on Grid Applications at GGF10, 2004.

D. P. Schissel, et al., *"Building the U.S. National Fusion Grid: Results from the National Fusion Collaboratory Project,"* The 4th IAEA Technical Meeting on Control, Data Acquisition, and Remote Participation for Fusion Research. Fusion Engineering and Design **71**, 245-250, 2004.

W. Schroers, et al. (The LHPC Collaboration), *"Moments of nucleon spin-dependent generalized parton distributions,"* Nuclear Physics (Proc. Suppl.) 129-130, 907, 2004.

W. H. Schubert, *"Generalization of Ertel's potential vorticity to a moist atmosphere,"* Meteorologische Zeitschrift, **13**, (Hans Ertel Special Issue), 465, 2004.

G. Schussman and K.-L. Ma, *"Anisotropic Volume Rendering for Extremely Dense, Thin Line Data,"* Proc. of the IEEE Visualization 2004 Conference, Austin, Texas, Oct. 2004.

S. L. Scott, C. B. Leangsuksun, T. Roa, J. Xu, and R. Libby, *"Experiments and Analysis towards effective cluster management system,"* 2004 High Availability and Performance Workshop (HAPCW), Santa Fe, NM, Oct. 2004.

S. L. Scott, C. Leangsuksun, T. Lui and R. Libby, *"HA-OSCAR Release 1.0 Beta: Unleashing HA-Beowulf,"* Proc.of 2nd Annual OSCAR Symposium, Winnipeg, Manitoba Canada, May 2004.

S. L. Scott, I. Haddad and C. Leangsuksun, *"HA-OSCAR: Towards Highly Available Linux Clusters,"* Linux World Magazine, **2,** 3, March 2004.

M. S. Shephard, M. W. Beall, R. M. O'Bara, B. E. Webster, *"Toward simulation-based design,"* Finite Elements in Analysis and Design, **40**, p. 1575-1598, 2004.

M. S. Shephard, M. W. Beall, B. E. Webster, *"Supporting Simulations to Guide Engineering Design,"* AIAA-2004-4448, AIAA, Richmond, Va., 2004.

J. Shigemitsu, et al. (The HPQCD collaboration), *"Heavy-light Meson Semileptonic Decays with Staggered Light Quarks,"* Nuclear Physics (Proc. Suppl.) 129-130, 331, 2004.

L. O. Silva et al., *"Proton shock acceleration in laser-plasma interactions,"* Physical Review Letters, **92**, 015002, 2004.

F. Song, F. Wolf, N. Bhatia, J. Dongarra, S. Moore, *"An Algebra for Cross-Experiment Performance Analysis,"* 2004 International Conference on Parallel Processing (ICCP-04), Montreal, Quebec, Canada, Aug. 2004.

C. R. Sovinec, A. H. Glasser, D. C. Barnes, T. A. Gianakon, R. A. Nebel, S. E. Kruger, D. D. Schnack, S. J. Plimpton, A. Tarditi, M. S. Chu and the NIMROD Team, *"Nonlinear magnetohydrodynamics with high-order finite elements,"* Journal Of Computational Physics **195**, 355, 2004.

H. R. Strauss, A. Pletzer, W. Park, S. Jardin, J. Breslau, and L. Sugiyama, *"MHD simulations with resistive wall and magnetic separatrix,"* Computer Physics Communications **164**, 1-3 40-45, 2004.

H. R. Strauss, L. Sugiyama, G. Y. Fu, W. Park, J. Breslau, *"Simulation of two fluid and energetic particle effects in stellarators,"* Nuclear Fusion **44**, 9, 1008-1014, 2004.

M. M. Strout and P. D. Hovland, *"Metrics and Models for Reordering Transformations,"* Proc. of the Second ACM SIGPLAN Workshop on Memory System Performance (MSP), June 2004.

M. M. Strout and P. D. Hovland, *"Metrics and Models for Reordering Transformations,"* Proc. of the Second ACM SIGPLAN Workshop on Memory System Performance (MSP), June 2004.

F. D. Swesty, E. S. Myra, *"Advances in Multi-Dimensional Simulation of Core-Collapse Supernovae,"* in Open Issues in Core Collapse Supernova Theory, Proc. of the Institute for Nuclear Theory, Vol. **14**, p. 176, University of Washington, Seattle, Wash., June 2004.

T. J. Tautges, *"MOAB-SD: Integrated Structured and Unstructured Mesh Representation,"* Engineering With Computers, **20**:286-293, 2004.

S. Thompson, B. Govindasamy, A. Mirin, K. Caldeira, C. Delire, J. Milovich, M. Wickett and D. J. Erickson III, *"Quantifying the effects of CO2-fertilized vegetation on future global climate and carbon dynamics,"* Geophysical Research Letters, **31**, L23211, 2004.

M. M. Tikir, J. K. Hollingsworth, *"Using Hardware Counters to Automatically Improve Memory Performance,"* Proc. of ACM/IEEE SC2004 conference, Pittsburgh, Penn., Nov. 2004.

J. L. Tilson, C. Naleway, M. Seth, R. Shepard, A. F. Wagner, and W. C. Ermler, *"An Ab Initio Study of AmCl+: f-f Spectroscopy and Chemical Binding,"* Journal of Chemical Physics, **121**, 5661-5675, 2004.

A. Toselli and O. Widlund, *"Domain Decomposition Methods - Algorithms and Theory,"* Springer Series in Computational Mathematics, **34**, Oct. 2004.

H. D. Trottier, *"Higher-order perturbation theory for highly-improved actions,"* Nuclear Physics (Proc. Suppl.) 129-130, 142, 2004.

F. S. Tsung et al., *"Near-GeV-energy laser-wakefield acceleration of self-injected electrons in a centimeter-scale channel"* Physical Review Letters **93**, 185002, 2004.

S. Vadlamani, S. E. Parker, Y. Chen, *"The Particle-Continuum method: an algorithmic unification of particle-in-cell and continuum methods,"* Computer Physics Communications, **164**, 209, 2004.

J.-L. Vay, P. Colella, J. W. Kwan, P. McCorquodale, D. B. Serafini, A. Friedman, D. P. Grote, G. Westenskow, J. C. Adam, A. Héron and I. Haber, *"Application of adaptive mesh refinement to particle-in-cell simulations of plasmas and beams,"* Physics of Plasmas **11**, 2928, 2004.

J-L. Vay, P. Colella, A. Friedman, D. P. Grote, P. McCorquodale, D. B. Serafini, *"Implementations of mesh refinement schemes*

for particle-in-cell plasma simulations," Computer Physics Communications **164**, p. 297-305, 2004.

M. Vertenstein, K. Oleson, S. Levis, and F. M. Hoffman, *"Community Land Model Version 3.0 (CLM3.0) User's Guide,"* National Center for Atmospheric Research, June 2004.

R. Vuduc, J. W. Demmel and J. A. Bilmes, *"Statistical Models for Empirical Search-Based Performance Tuning,"* International Journal of High Performance Computing Applications, **18** (1), p. 65-94, February 2004.

G. Wallace, et al., *"Automatic Alignment of Tiled Displays for a Desktop Environment,"* Journal of Software. **15**(12): 1776-1786, Dec. 2004.

W. X. Wang, et al., *"Global delta-f particle simulation of neoclassical transport and ambipolar electric field in general geometry,"* Computer Physics Communications, **164**, 178, 2004.

T. P. Wangler, C. K. Allen, K. C. D. Chan, P. L. Colestock, K. R. Crandall, R. W. Garnett, J. D. Gilpatrick, W. Lysenko, J. Qiang, J. D. Schneider, M. E. Schulze, R. L. Sheffield, H. V. Smith, *"Beam-Halo in Mismatched Proton Beams,"* Instrument Methods Physics Res. A **519**, 425, 2004.

J. Wei, A. Fedotov, W. Fischer, N. Malitsky, G. Parzen, J. Qiang, *"Intra-beam Scattering Theory and RHIC Experiments,"* Proc. 33rd ICFA Advanced Beam Dynamics Workshop on High Intensity & High Brightness Hadron Beams, Bensheim, Germany, Oct. 2004.

M. Wingate, et al. (The HPQCD collaboration), *"Progress Calculating Decay Constants with NRQCD and AsqTad actions,"* Nuclear Physics (Proc. Suppl.) 129-130, 325, 2004.

M. Wingate, et al. (The HPQCD Collaboration), *"The Bs and Ds decay constants in 3 flavor lattice QCD,"* Physical Review Letters **92**, 162001, 2004.

F. Wolf, B. Mohr, J. Dongarra, S. Moore, *"Efficient Pattern Search in Large Traces through Successive Refinement,"* Proc. of Euro-Par 2004, Pisa, Italy, Aug.-Sept. 2004.

S. E. Woosley, A. Heger, A. Cumming, R. D. Hoffman, J. Pruet, T. Rauscher, J. L. Fisker, H. Schatz, B. A. Brown and M. Wiescher, *"Models for Type I X-Ray Bursts with Improved Nuclear Physics,"* Astrophysical Journal Supplement, **151**:75-102, March 2004.

S. E. Woosley, S. Wunsch and M. Kuhlen, *"Carbon Ignition in Type Ia Supernovae: An Analytic Model,"* Astrophysical Journal, **607**:921-930, June 2004.

P. H. Worley, J. Levesque, *"The Performance Evolution of the Parallel Ocean Program on the Cray X1,"* Proc. of the 46th Cray User Group Conference, Knoxville, TN, May 2004.

J. C. Wright, P. T. Bonoli, M. Brambilla, F. Meo, E. D'Azevedo, D. B. Batchelor, E. F. Jaeger, L. A. Berry, C. K. Phillips and A. Pletzer, *"Full Wave Simulations of Fast Wave Mode Conversion and Lower Hybrid Wave Propagation in Tokamaks,"* Physics of Plasmas **11**, 2473, 2004.

J. C. Wright, P. T. Bonoli, E. D'Azevedo and M. Brambilla, *"Ultrahigh resolution simulations of mode converted ion cyclotron waves and lower hybrid waves,"* Proc. of the 18th International Conference on the Numerical Simulation of Plasmas, Computer Physics Communications **164**, 330, 2004.

K. Wu, J. Ekow, E. J. Otoo, and A. Shoshani, *"On the performance of bitmap indices for high cardinality attributes,"* Proc. of the Thirtieth International Conference on Very Large Data Bases, Toronto, Canada, Morgan Kaufmann, Sept. 2004.

K. Wu, W.-M. Zhang, V. Perevoztchikov, J. Lauret and A. Shoshani, *"The grid collector: Using an event catalog to speed up user analysis in distributed environment,"* Proc. of Computing in High Energy and Nuclear Physics (CHEP), Interlaken, Switzerland, Sept. 2004.

S. Wunsch and S. E. Woosley, *"Convection and Core-Center Ignition in Type Ia Supernovae,"* Astrophysical Journal, **616**:1102-1108, Dec. 2004.

D. Xu and B. Bode, *"Performance Study and Dynamic Optimization Design for Thread Pool Systems,"* Proc. of the International Conference on Computing, Communications and Control Technologies (CCCT'2004), Austin, Texas, Aug. 2004.

C. Yang, W. Gao, Z. Bai, X. Li, L. Lee, P. Husbands and E. Ng., *"Algebraic Sub-structuring for Large-scale Electromagnetic Applications,"* PARA'04 Workshop on State-of-the-art in Scientific Computing, Copenhagen, Denmark, June 2004.

U. M. Yang, *"On the Use of Relaxation Parameters in Hybrid Smoothers,"* Numer. Linear Algebra Appl., **11**, p. 155-172, 2004.

Q. Yi, K. Kennedy, H. You, K. Seymour, and J. Dongarra, *"Automatic Blocking of QR and LU Factorizations for Locality,"* Second ACM SIGPLAN Workshop on Memory System Performance, Washington, D.C., June 2004.

Q. Yi and D. Quinlan, *"Applying Loop Optimizations to Object-Oriented Abstractions Through General Classification of Array Semantics,"* 17th International Workshop on Languages and Compilers for Parallel Computing, West Lafayette, Ind., Sept. 2004.

H. Yu, K.-L. Ma and J. Welling, *"A Parallel Visualization Pipeline for Terascale Earthquake Simulations,"* Proc. of the ACM/IEEE SC04 conference, Pittsburgh, Penn., Nov. 2004.

H. Yu, K.-L. Ma and J. Welling, *"I/O Strategies for Parallel Rendering of Large Time-Varying Volume Data,"* Proc. of the Eurographics/ACM SIGGRAPH Symposium on Parallel Graphics and Visualization, June 2004.

O. Zatsarinny, T. W. Gorczyca, K. T. Korista, N. R. Badnell and D. W. Savin, *"Dielectronic recombination data for dynamic finite-density plasmas: IV. The Carbon iso-electronic sequence,"* Astronomy and Astrophysics, **417**, 1173, 2004.

H. Zhang, et al., *"Providing Data Transfer with QoS as Agreement-Based Service,"* Proc. of the IEEE International Conference on Services Computing, 2004.

W. Zhang, S. E. Woosley and A. Heger, *"The Propagation and Eruption of Relativistic Jets from the Stellar Progenitors of Gamma-Ray Bursts,"* Astrophysical Journal, **608**:365-377, June 2004.

2005–2006

G. Abla, et al., *"Shared Display Wall Based Collaboration Environment in the Control Room of the DIII-D National Fusion Facility,"* Fifth Annual Workshop on Advanced Collaborative Environments (WACE2005), 2005.

G. Abla, et al., *"Advanced Tools for Enhancing Control Room Collaborations,"* The 5th IAEA Technical Meeting on Control, Data Acquisition, and Remote Participation for Fusion Research, 2005.

Mark Adams, *"Ax=b: The Link Between Gyrokinetic Particle Simulations of Turbulent Transport in Burning Plasmas and Micro-FE Analysis of Whole Vertebral Bodies in Orthopaedic Biomechanics,"* invited talk, SciDAC Conference, San Francisco, Calif., June 2005.

C. M. Aikens, G. D. Fletcher, M. W. Schmidt and M. S. Gordon, *"Scalable Implementation Of Analytic Gradients For Second-Order Z-Averaged Perturbation Theory Using The Distributed Data Interface,"* Journal of Chemical Physics., **124**, 014107, 2006.

V. Akcelik, J. Bielak, I. Epanomeritakis, O. Ghattas and E. Kim, *"High fidelity forward and inverse earthquake modeling in large basins,"* Proc. of the Sixth European Conference on Structural Dynamics EURODYN'05, Paris, France, Sept. 2005.

V. Akcelik, G. Biros, A. Dragenescu, J. Hill, O. Ghattas and B. van Bloemen Waanders, *"Dynamic data-driven inversion for terascale simulations: Real-time identification of airborne contaminants,"* Proc. of, ACM/IEEE SC2005 conference, Seattle, Wash., Nov. 2005.

V. Akcelik, G. Biros, O. Ghattas, D. Keyes, K. Ko, L.-Q. Lee and E. Ng, *"Adjoint Methods For Electromagnetic Shape Optimization Of The Low-Loss Cavity For The International Linear Collider,"* Proc. of SciDAC 2005 Conference, San Francisco, Calif., June 2005.

V. Akcelik, G. Biros, O. Ghattas, D. Keyes, K. Ko, L.-Q. Lee and E. G. Ng, *"Adjoint Methods for Electromagnetic Shape Optimization of the Low-Loss Cavity for the International Linear Collider,"* Proc. of SciDAC 2005, San Francisco, Calif., June 2005.

V. Akcelik, G. Biros, O. Ghattas, J. Hill, D. Keyes, and B. van Bloeman Waanders, *"Parallel PDE constrained optimization,"* in Frontiers of Parallel Computing, M. Heroux, P. Raghaven, and H. Simon, eds, SIAM, to appear 2006.

H. Akiba, K.-L. Ma, and J. Clyne, *"End-to-end Data Reduction and Hardware Accelerated Rendering Techniques for Visualizing Time-Varying Non-uniform Grid Volume Data,"* Proc. of the International Workshop on Volume Graphics 2005, Stony Brook, NY, June 2005.

M. A. Albao, D.-J. Liu, C. H. Choi, M. S. Gordon and J. W. Evans, *"Competitive Etching and Oxidation of Vicinal Si(100) Surfaces,"* MRS Proceedings Vol. **85**9E, JJ3.6., 2005.

M. A. Albao, M. M. R. Evans, J. Nogami, D. Zorn, M. S. Gordon and J. W. Evans, *"Atomistic processes mediating growth of one-dimensional Ga rows on Si(100),"* Physical Review B **72**, 035426, 2005.

M. A. Albao, D.-J. Liu, M. S. Gordon and J. W. Evans, *"Simultaneous Etching and Oxidation of Vicinal Si(100) Surfaces: Atomistic Lattice-Gas Modeling of Morphological Evolution,"* Physical Review B **72**, 195420, 2005.

A. Alexandru, et al., *"Progress on a Canonical Finite Density Algorithm,"* Nuclear Physics B (Proc. Suppl.) **140**, 517, 2005.

C. Alexandru, et al. (The LHPC Collaboration), *"First principles calculations of nucleon and pion form factors: Understanding the building blocks of nuclear matter from lattice QCD,"* Journal of Physics Conf. Ser. **16**, 174, 2005.

C. Alexandrou, et al., *"Momentum dependence of the N to Delta transition form factors,"* Nuclear Physics B (Proc. Suppl.) **140**, 293, 2005.

I. F. Allison et al. (The HPQCD Collaboration), *"Mass of the B/c meson in three-flavor lattice QCD,"* Physical Review Letters **94**, 172001, 2005.

I. F. Allison et al. (The HPQCD Collaboration), *"A precise determination of the B/c mass from dynamical lattice QCD,"* Nuclear Physics (Proc. Suppl.) **140**, 440, 2005.

A. S. Almgren, J. B. Bell, C. A. Rendleman, and M. Zingale, *"Low Mach Number Modeling of Type Ia Supernovae,"* ApJ, **637**, 922, 2006.

J. Amundson, P. Spentzouris, *"Space charge experiments and simulation in the Fermilab Booster,"* Proc. of Particle Accelerator Conference (PAC 05), Knoxville, Tenn., May 2005.

J. Amundson, P. Spentzouris, J.Qiang and R. Ryne, *"Synergia: An accelerator modeling tool with 3-D space charge,"* Journal of Computational Physics vol. **211**, 229, 2006.

A. Andrady, P. J. Aucamo, A. F. Bais, C. L. Ballare, L. O. Bjorn, J. F. Bornman, M. Caldwell, A. P. Cullen, D. J. Erickson III, F. R. de Gruijl, D.-P. Hader, M. ilyas, G. Kulandaivelu, H. D. Kumar, J. Longstreth, R. L. McKenzie, M. Norval, H. H. Redhwi, R. C. Smith, K. R. Solomon, Y. Takizawa, X. Tang, A. H. Teramura, A. Torikai, J. C. van der Leun, S. Wilson, R. C. Worrest and R. G. Zepp, *"Environmental effects of ozone depletion and its interactions with climate change: Progress Report 2004,"* Photochem. Photobiol. Sci., 2005.

D. J. Antonio et al. (The RBC and UKQCD Collaborations), *"Baryons in 2+1 flavour domain wall QCD,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 098, 2005.

C. Aubin, et al. (The MILC Collaboration), *"Properties of light quarks from lattice QCD simulations,"* Journal of Physics: Conference Proceedings, **16**, 160, 2005.

C. Aubin, et al. (The Fermilab Lattice, MILC, and HPQCD Collaborations), *"Semileptonic decays of D mesons in three-flavor lattice QCD,"* Physical Review Letters **94**, 011601, 2005.

C. Aubin, et al. (The Fermilab Lattice, MILC, and HPQCD Collaborations), *"Charmed meson decay constants in three flavor lattice QCD,"* Physical Review Letters **95**, 122002, 2005.

C. Aubin, et al. (The MILC Collaboration), *"Topological susceptibility with three flavors of staggered quarks,"* Nuclear Physics. B (Proc. Suppl.) **140**, 600, 2005.

C. Aubin, et al. (The MILC Collaboration), *"Results for light pseudoscalars from three-flavor simulations,"* Nuclear Physics. B (Proc. Suppl.) **140**, 231, 2005.

C. Aubin, et al. (The MILC Collaboration), *"The scaling dimension of low lying Dirac eigenmodes and of the topological charge density,"* Nuclear Physics. B (Proc. Suppl.) **140**, 626, 2005.

B. Bader, O. Ghattas, B. van Bloemen Waanders and K. Willcox, *"An optimization framework for goal-oriented model-based reduction of large-scale systems,"* 44th IEEE Conference on Decision and Control, Seville, Spain, Dec. 2005.

D. H. Bailey and A. S. Snavely, *"Performance Modeling: Understanding the Present and Predicting the Future,"* Proc. of SIAM PP04, 2005.

A. H. Baker, E. R. Jessup, and T. A. Manteuffel, *"A technique for accelerating the convergence of GMRES,"* SIAM J. Mat. Anal. & App., **26**, 4, p. 962, 2005.

S. Basak, et al., *"Combining quark and link smearing to improve extended baryon operators,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), **076**, 2005.

S. Basak, et al. (The LHPC Collaboration), *"Baryonic sources using irreducible representations of the double-covered octahedral group,"* Nuclear Physics. (Proc. Suppl.) **140**, 281, 2005.

S. Basak, et al. (The LHPC Collaboration), *"Analysis of N* spectra using matrices of correlation functions based on irreducible baryon operators,"* Nuclear Physics (Proc. Suppl.) **140**, 278, 2005.

S. Basak, et al. (The LHPC Collaboration), *"Group-theoretical construction of extended baryon operators,"* Nuclear Physics. (Proc. Suppl.) **140**, 287, 2005.

S. Basak, et al. (The LHPC Collaboration), *"Group-theoretical construction of extended baryon operators in lattice QCD,"* Physical Review D, **72**, 094506, 2005.

S. Basak, et al. (The LHPC Collaboration), *"Clebsch-Gordan construction of lattice interpolating fields for excited baryons,"* Physical Review D, **72**, 074501, 2005.

A. C. Bauer, M. S. Shephard, M., Nuggehally, *"Design overview of the TSTT integrated field approximation for numerical simulation (FANS) library,"* Proc. 8th US Nat. Congress on Comp. Mech., 2005.

J. B. Bell, M. S. Day, J. F. Grcar, and M. J. Lijewski, *"Active Control for Statistically Stationary Turbulent Premixed Flame Simulations,"* Communications in Applied Mathematics and Computational Science, **1**, 29, 2006.

J. B. Bell, M. S. Day, I. G. Shepherd, M. Johnson, R. K. Cheng, J. F. Grcar, V. E. Beckner, and M. J. Lijewski, *"Numerical Simulation of a Laboratory-Scale Turbulent V- flame,"* Proceedings of the National Academy of Sciences, **102** (29) 10006, 2005.

G. J. O. Beran, B. Austin, A. Sodt, and M. Head-Gordon, *"Unrestricted perfect pairing: The simplest wave-function-based model chemistry beyond mean field,"* Journal of Physical Chemistry A, **109**, 9183-9192, 2005.

C. Bernard, et al. (The MILC Collaboration), *"The locality of the fourth root of staggered fermion determinant in the interacting case,"* XXIII International Symposium on Lattice Field Theory (Lattice 2005), 299, 2005.

C. Bernard, et al. (The MILC Collaboration), *"More evidence of localization in the low-lying Dirac spectrum,"* XXIII International Symposium on Lattice Field Theory (Lattice 2005), 299, 2005.

C. Bernard, et al. (The MILC Collaboration), *"The Equation of State for QCD with 2+1 Flavors of Quarks,"* Proceedings of Science, Lattice 2005, 156, 2005.

C. Bernard, et al. (The MILC Collaboration), *"Update on pi and K Physics,"* XXIII International Symposium on Lattice Field Theory (Lattice 2005), 025, 2005.

C. Bernard, et al. (TheMILC Collaboration), *"QCDThermodynamics with Three Flavors of Improved Staggered Quarks,"* Physical Review D, **71**, 034504, 2005.

C. Bernard, et al. (The MILC Collaboration), *"Heavy-light decay constants using clover valence quarks and three flavors of dynamical improved staggered quarks,"* Nuclear Physics. B (Proc. Suppl.) **140**, 449, 2005.

C. Bernard, et al. (The MILC Collaboration), *"Three Flavor QCD at High Temperatures,"* Nuclear Physics B (Proc. Suppl.) **140**, 538, 2005.

M. Berndt, T. Manteuffel, and S. McCormick, and G. Starke, *"Analysis of first-order system least squares (FOSLS) for elliptic problems with discontinuous coefficients: Part I,"* SIAM Journal on Numerical Analysis, **43**, p. 386-408, 2005.

M. Berndt, T. Manteuffel and S. McCormick, *"Analysis of first-order system least squares (FOSLS) for elliptic problems with discontinuous coefficients: Part II,"* SIAM Journal on Numerical Analysis, **43**, p. 409-436, 2005.

M. Barad, P. Colella, *"A fourth-order accurate local refinement method for Poisson's equation,"* J. Comput. Phys. **209**, p. 1-18, 2005.

N. Bhatia, F. Song, F. Wolf, J. Dongarra, B. Mohr, S. Moore, *"Automatic Experimental Analysis of Communication Patterns in Virtual Topologies,"* Proc. of the International Conference on Parallel Processing (ICPP-05), Oslo, Norway, June 2005.

B. Bhattacharjee, P. Lemonidis, W. H. Green, and P. I. Barton, *"Global Solution of Semi-Infinite Programs,"* Mathematical Programming, **103**, 283, 2005.

G. Biros and O. Ghattas, *"Parallel Lagrange-Newton-Krylov-Schur Methods for PDE-Constrained Optimization. Part I: The Krylov-Schur Solver,"* SIAM Journal on Scientific Computing, **27**, 687, 2005.

G. Biros and O. Ghattas, *"Parallel Lagrange-Newton-Krylov-Schur Methods for PDE-Constrained Optimization. Part II: The Lagrange-Newton Solver, and its Application to Optimal Control of Steady Viscous Flows,"* SIAM Journal on Scientific Computing, **27**, 714, 2005.

B. Bistrovic, et al. (The LHPC Collaboration), *"Understanding hadron structure from lattice QCD in the SciDAC era,"* Journal of Physics Conf. Ser. **16**, 150, 2005.

J. M. Blondin, *"Discovering new dynamics of core-collapse supernova shock waves,"* Journal of Physics Conference Series, **16**, 370-379, 2005.

J. M. Blondin, A. Mezzacappa, *"The Spherical Accretion Shock Instability in the Linear Regime,"* ArXiv Astrophysics e-prints, July 2005.

T. Blum, *"Lattice calculation of the lowest-order hadronic contribution to the muon anomalous magnetic moment,"* Nuclear Physics B (Proc. Suppl.) **140**, 311, 2005.

T. Blum and P. Petreczky, *"Cutoff effects in meson spectral functions,"* Nuclear Physics B (Proc. Suppl.) **140**, 553, 2005.

F.D.R. Bonnet, et al. (The LHPC Collaboration), *"Lattice computations of the pion form factor,"* Phys. Rev. D **72**, 054506, 2005.

P. A. Boyle, et al., *"Overview of the QCDSP and QCDOC computers,"* IBM Research Journal **49**, 351, 2005.

P. A. Boyle, et al., *"QCDOC: Project status and first results,"* Journal of Physics Conf. Ser. 16, 129, 2005.

P. A. Boyle, et al., *"Localisation and chiral symmetry in 2+1 flavour domain wall QCD,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 141, 2005.

P. A. Boyle, et al., *"The QCDOC project,"* Nuclear Physics (Proc. Suppl.) **140**, 169, 2005.

J. Brannick, M. Brezina, S. MacLachlan, T. Manteuffel, S. McCormick, and J. Ruge, *"An energy-based AMG coarsening strategy,"* Journal on Numerical Analysis,. Lin. Alg. Appl., **13**, 133, 2006.

D. P. Brennan, S. E. Kruger, T. A. Gianakon, and D. D. Schnack, *"A categorization of tearing mode onset in tokamaks via nonlinear simulation,"* Nuclear Fusion **45**. 1178, 2005.

M. Brezina, R. Falgout, S. MacLachlan, T. Manteuffel, S. McCormick and J. Ruge, *"Adaptive Smoothed Aggregation (_SA),"* SIAM Review: SIGEST, **47**, p. 317, 2005.

M. Brezina, R. Falgout, S. MacLachlan, T. Manteuffel, S. McCormick and J. Ruge, *"Adaptive Algebraic Multigrid,"* SIAM Journal of Scientific Computing, **27**, 1534, 2006.

M. Brezina, C. Tong, R. Becker, *"Parallel Algebraic Multigrids for Structural Mechanics,"* SIAM Journal of Scientific Computing, to appear.

R. C. Brower, H. Neff, and K. Orginos, *"Moebius fermions: Improved domain wall chiral fermions,"* Nuclear Physics. (Proc. Suppl.) **140**, 686, 2005.

J. R. Burruss, et al., *"Security on the U. S. Fusion Grid,"* The 5th IAEA Technical Meeting on Control, Data Acquisition, and Remote Participation for Fusion Research, 2005.

J. R. Burruss, et al., *"Simplifying FusionGrid Security,"* Proc. Challenges of Large Applications in Distributed Environments, 95-105, 2005.

J. R. Burruss, *"The Resource Oriented Authorization Manager (ROAM),"* Proc. 14th IEEE International Symposium on High Performance Distributed Computing, 308-309, 2005.

J. R. Burruss, et al., *"Developments in Remote Collaboration and Computation,"* The 14th ANS Topical Meeting on the Technology of Fusion Energy, Fusion Science and Technology, **47**, 3, 814, 2005.

L. Bytautas and K. Ruedenberg, *"Correlation Energy Extrapolation through Intrinsic Scaling. IV. Accurate Binding Energies of the Homonuclear Diatomic Molecules Carbon, Nitrogen, Oxygen and Fluorine,"* Journal of Chemical Physics, **122**, 154110, 2005.

X.-C. Cai, L. Marcinkowski, and P. Vassilevski, "An element agglomeration nonlinear additive Schwarz preconditioned Newton method for unstructured finite element problems," Applications of Mathematics, **50**, p. 247-275, 2005.

C. Y. Cardall, E. J. Lentz, A. Mezzacappa, *"Conservative special relativistic radiative transfer for multidimensional astrophysical simulations: Motivation and elaboration,"* Physical Review D, **72**, 043007, 2005.

C. Y. Cardall, A. O. Razoumov, E. Endeve, E. J. Lentz, A. Mezzacappa, *"Toward five-dimensional core-collapse supernova simulations,"* Journal of Physics Conference Series, **16**, 390-394, 2005.

G. R. Carr, M. J. Cordery, J. B. Drake, M. W. Ham, F. M. Hoffman and P. H. Worley, "Porting and Performance of the Community Climate System Model (CCSM3) on the Cray X1," Proc. of the 47th Cray User Group Conference, Albuquerque, NM, May 2005.

L. Carrington, M. Laurenzano, A. Snavely, R. Campbell and L. Davis, *"How well can simple metrics represent the performance of HPC applications?"* Proc. of the ACM/IEEE SC05 conference, Seattle, Wash., Nov. 2005.

T. Chartier, R. Falgout, V. E. Henson, J. Jones, T. Manteuffel, S. McCormick, J. Ruge and P. Vassilevski, *"Spectral element agglomerate AMGe,"* Lecture Notes in Computational Science and Engineering, to appear.

J. Chen, S. C. Jardin, and H. R. Strauss, *"Solving anisotropic transport equations on misaligned grids,"* Lecture Notes In Computer Science, **3516**, 1076-1079, 2005.

J. Chen, J. Breslau, G. Fu, S. Jardin, W. Park, *"Symmetric solution in M3D,"* Computer Physics Communications **164**, 1-3, 468-471, 2005.

H. Chen, et al., *"Memory Performance Optimizations for Real-Time Software HDTV Decoding,"* The Journal of VLSI Signal Processing, **21**, 2, 193-207, 2005.

L. Chen, F. Zonca, and Z. Lin, *"Nonlinear Toroidal Mode Coupling: A New Paradigm for Drift Wave Turbulence in Toroidal Plasmas,"* Plasma Phys. Contr. Fusion **47**, B71, 2005.

M. Cheng, et al. (The RBC-Bielefeld Collaboration), *"Scaling test of the P4-improved staggered fermion action,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 045, 2005.

N. Chevaugeon, P. Hu, X. Li, J. Xin, D. Cler, J. E. Flaherty, M. S. Shephard, *"Discontinuous Galerkin methods applied to shock and blast problems,"* Journal of Scientific Computing, **22**, p. 227-243, 2005.

E. Chow, *"An Aggregation Multilevel Method Using Smooth Error Vectors,"* SIAM Journal of Scientific Computing, **27**, 1727, 2006.

M. Choi, V. S. Chan, V. Tang, P. Bonoli, R. I. Pinsker, *"Monte-Carlo Orbit/Full Wave Simulation of Fast Alfvén (FW) Damping on Resonant Ions in Tokamaks,"* Radio Frequency Power in Plasmas, Proc. 16th Topical Conf., Park City, Utah, 2005.

M. A. Clark, P. de Forcrand and A. D. Kennedy, *"Algorithm shootout: R versus RHMC,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 115, 2005.

C. S. Co, A. Friedman, D. P. Grote, J.-L.Vay, W. Bethel, K. I. Joy, *"Interactive Methods for Exploring Particle Simulation Data,"* Proc. of EuroVis 2005 conference, 2005.

B. Cohen, E. B. Hooper, R. H. Cohen, D. N. Hill, H. S. McLean, R. D. Wood, S. Woodruff, C. R. Sovinec, and G. A. Cone, *"Simulation of spheromak evolution and energy confinement,"* Physics of Plasmas, **12**, 056106, 2005.

S. Cohen, *"Preliminary Study of BK on 2+1 flavor DWF lattices from QCDOC,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 346, 2005.

P. Colella, D. T. Graves, B. J. Keen, D. Modiano, *"A cartesian grid embedded boundary method for hyperbolic conservation laws,"* Journal of Computational Physics, **211**, p. 347-366, 2006.

I. R. Corey, J. R. Johnson and J. S. Vetter, *"Performance Assertions and Sensitivity*

Analysis: A Technique for Developing Adaptive Grid Applications," Proceedings of the Eleventh IEEE International Symposium on High Performance Distributed Computing, (HPDC), Edinburgh, Scotland, July 2006.

A. P. Craig, R. L. Jacob, B. Kauffman, T. Bettge, J. Larson, E. Ong, C. Ding, and Y. He, *"CPL6: The New Extensible, High-Performance Parallel Coupler for the Community Climate System Model,"* International Journal of High Performance Computing Applications, **19**, 3, p. 309, Aug. 2005.

R. K. Crockett, P. Colella, R. Fisher, R. I. Klein, C. F. McKee, *"An unsplit, cell-centered Godunov method for ideal MHD,"* J. Comput. Phys. **203**, p. 422-448, 2005.

C.T.H. Davies, G. P. Lepage, F. Niedermayer and D. Toussaint, (The HPQCD, MILC and UKQCD Collaborations), *"The Quenched Continuum Limit,"* Nuclear Physics B (Proc. Suppl.) **140**, 261, 2005.

M. S. Day, J. B. Bell, J. F. Grcar, and V. E. Beckner, *"Numerical Control of 3D Turbulent Premixed Flame Simulations,"* 20th International Colloquium on the Dynamics of Explosions and Reactive Systems, July-Aug, 2005.

H. de Sterck, T. Manteuffel, S. McCormick and L. Olson, *"Numerical conservation properties of H(div)-conforming least-squares finite element methods for the Burgers equation,"* SIAM Journal of Scientific Computing, **26**, p. 1573-1597, 2005.

H. de Sterck, R. Markel and R. Knight, *"TaskSpaces: a software framework for parallel bioinformatics on computational grids,"* in Parallel Computing in Bioinformatics and Computational Biology, A. Zomaya, editor, J. Wiley and Sons, 2005.

J. Demmel, J. Dongarra, V. Eijkhout, E. Fuentes, A. Petitet, R. Vuduc, R. C. Whaley, and K. Yelick, *"Self-Adapting Linear Algebra Algorithms and Software,"* Proc. of the IEEE, Special Issue on Program Generation, Optimization, and Platform Adaptation, **93**(2), Feb. 2005.

N. Desai, R. Bradshaw, S. Matott, S. Bittner, S. Coghlan, R. Evard, C. Luenighoener, T. Leggett, J. P. Navarro, G. Rackow, C. Stacey, and T. Stacey, *"A case study in configuration management tool deployment,"* Proc. of the Nineteenth System Administration Conference (LISA XIX), San Diego, Calif., Dec. 2005.

N. Desai, A. Lusk, R. Bradsha, and E. Lusk, *"{MPISH}: A parallel shell for {MPI} programs,"* Proc. of the 1st Workshop on System Management Tools for Large-Scale Parallel Systems (IPDPS '05), Denver, Colo., 2005.

Z. M. Djurisic, D. Amusin, T. Bereknyei, T. C. Allison, M. Frenklach, *"Reporting of experimental data for development and validation of chemical kinetic models,"* Fall Meeting of the Western States Section of the Combustion Institute, Stanford, CA, Oct. 2005.

J. B. Drake, P. W. Jones, G. R. Carr Jr., *"Overview of the Software Design of the Community Climate System Model,"* International Journal of High Performance Computational Application, **19**, 177, 2005.

T. Draper, et al., *"Improved Measure of Local Chirality,"* Nuclear Physics B (Proc. Suppl.) **140**, 623, 2005.

T. Draper, et al., *"Locality and Scaling of Quenched Overlap Fermions,"* Draper, et al., Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), **120**, 2005.

H. Duan, G. M. Fuller, Y.-Z. Qian, *"Collective Neutrino Flavor Transformation In Supernovae,"* ArXiv Astrophysics e-prints, Nov. 2005.

J. Dudek, R. G. Edwards and D. G. Richards, *"Radiative transitions in charmonium,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 210, 2005.

T. J. Dudley, R. M. Olson, M. W. Schmidt, and M .S. Gordon, *"Parallel Coupled Perturbed CASSCF Equations and Analytic CASSCF Second Derivatives,"* Journal of Computational Chemistry, **27**, 352, 2006.

T. H. Dunigan, Jr., J. S. Vetter and P. H. Worley, *"Performance Evaluation of the SGI Altix 3700,"* Proc. of the 2005 International Conference on Parallel Processing, Oslo, Norway, June 2005.

T. H. Dunigan, Jr., J. S. Vetter, J. B. White III, and P. H. Worley, *"Performance Evaluation of the Cray X1 Distributed Shared-Memory Architecture,"* IEEE Micro, **25**(1), p. 30, Jan./Feb. 2005.

R. J. Dumont, C. K. Phillips and D. N. Smithe, *"Effects of non-Maxwellian species on ion cyclotron wave propagation and absorption in magnetically confined plasmas,"* Physics of Plasmas **12**, 042508, 2005.

R. G. Edwards, et al. (The LHPC Collaboration), *"Hadron structure with light dynamical quarks,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 056, 2005.

R. G. Edwards et al. (The LHPC and UKQCD Collaborations), *"The Chroma Software System for Lattice QCD,"* Nuclear Physics (Proc. Suppl.) **140**, 832, 2005.

S. Ethier, *"Gyrokinetic Particle-in-Cell Simulations of Plasma Microturbulence on Advanced Computing Platforms,"* keynote talk, SciDAC Conference, San Francisco 2005.

J. W. Evans, *"Kinetic Monte Carlo Simulation of Non-Equilibrium Lattice-Gas Models: Basic and Refined Algorithms applied to Surface Adsorption Processes,"* in Handbook of Materials Modeling, Part A, Ch. 5.12, ed. S. Yip, Springer, Berlin, 2005.

M. R. Fahey, S. Alam, T. H. Dunigan, Jr., J. S. Vetter and P. H. Worley, *"Early Evaluation of the Cray XD1,"* Proc. of the 47th Cray User Group Conference, Albuquerque, NM, May 2005.

R. Falgout, J. Brannick, M. Brezina, T. Manteuffel, and S. McCormick, *"New multigrid solver advances in TOPS,"* Proceedings of SciDAC 2005, Journal of Physics: Conference Series, Institute of Physics, San Francisco, Calif., June 2005.

R. D. Falgout, J. E. Jones, and U. M. Yang, *"The Design and Implementation of hypre, a Library of Parallel High Performance Preconditioners,"* chapter in Numerical Solution of Partial Differential Equations on Parallel Computers, A. M. Bruaset, P. Bjørstad, and A. Tveito, eds., Springer-Verlag, 2006.

R. D. Falgout, J. E. Jones, and U. M. Yang, *"Conceptual Interfaces in hypre,"* Future Generation Computer Systems, Special Issue on PDE software, **22**, p. 239-251, 2005.

R. D. Falgout, J. E. Jones and U. M. Yang, *"Pursuing Scalability for hypre's Conceptual Interfaces,"* ACM Transactions of Mathematical Softw., **31**, p. 326-350, 2005.

R. D. Falgout, P. S. Vassilevski, and L. T. Zikatanov, *"On Two-Grid Convergence Estimates,"* Numer. Linear Algebra Appl., **12**, p. 471-494, 2005.

D.G. Fedorov, K. Kitaura, H. Li, J. H. Jernsen, and M. S. Gordon, *"The polarizable continuum model (PCM) interfaced with the fragment molecular orbital method (FMO),"* Journal of Computational Chemistry, in press.

J. Feng, W. Wan, J. Qiang, A. Bartelt, A. Comin, A. Scholl, J. Byrd, R. Falcone, G. Huang, A. MacPhee, J. Nasiatka, K. Opachich, D. Weinstein, T. Young and H. A. Padmore, *"An Ultra-Fast X-Ray Streak Camera for the Study of Magnetication Dynamics,"* Proceedings of SPIE, 2005.

G. Fleming, et al. (The LHPC Collaboration), *"Pion form factor using domain wall valence and asqtad sea quarks,"* Nuclear Physics (Proc. Suppl.) 140, 302 2005.

G. Folatelli, C. Contreras, M. M. Phillips, S. E. Woosley, S. Blinnikov, N. Morrell, N. B. Suntzeff, B. L. Lee, M. Hamuy, S. Gonzalez, W. Krzeminski, M. Roth, W. Li, A. V. Filippenko, W. L. Freedman, B. F. Madore, S. E. Persson, D. Murphy, S. Boissier, G. Galaz, L. Gonzalez, P. J. McCarthy, A. McWilliam and W. Pych, *"SN 2005bf: A Transition Event Between Type Ib/c Supernovae and Gamma Ray Bursts,"* ArXiv Astrophysics e-prints, Sept. 2005.

I. Foster, *"Service-Oriented Science,"* Science Magazine, **308**, 5723, 814-817, May 2005.

N. Fout, H. Akiba, K.-L. Ma, A. Lefohn, and J. Kniss, *"High Quality Rendering of Compressed Volume Data Formats,"* Proc. of the Eurographics/IEEE-VGTC Symposium on Visualization (EuroVis 2005), Leeds, UK, June 2005.

N. Fout, K.-L. Ma, and J. Ahrens, *"Time-Varying Multivariate Volume Data Reduction,"* Proc. of the ACM Symposium on Applied Computing 2005, p. 1224-1230, Santa Fe, NM, March 2005.

C. L. Fryer and A. Heger, *"Binary Merger Progenitors for Gamma-Ray Bursts and Hypernovae,"* ApJ, **623**:302-313, April 2005.

C. L. Fryer, G. Rockefeller, A. Hungerford, and F. Melia, *"The Sgr B2 X-ray Echo of the Galactic Center Supernova Explosion that Produced Sgr A East,"* ArXiv Astrophysics e-prints, June 2005.

G. M. Fuller, Y.-Z. Qian, *"Simultaneous Flavor Transformation of Neutrinos and Antineutrinos with Dominant Potentials from Neutrino-Neutrino Forward Scattering,"* ArXiv Astrophysics e-prints, May 2005.

E. Gamiz, et al. (The HPQCD Collaboration), *"Dynamical Determination of BK from Improved Staggered Quarks,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 47 2005.

E. Gamiz, et al. (The HPQCD Collaboration), *"BK from Improved Staggered Quarks,"* Nuclear Physics (Proc. Suppl.) **140**, 353, 2005.

W. Gao, X. S. Li, C. Yang, Z. Bai, *"Performance Evaluation of a Multilevel Sub-structuring Method for Sparse Eigenvalue Problems,"* Proc. of the 16th International Conference on Domain Decomposition Methods, 2005.

X. Gao, B. Simon, and A. Snavely, *"ALITER: An Asynchronous Lightweight Instrumentation Tool for Event Recording,"* Workshop on Binary Instrumentation and Applications, St. Louis, Mo. Sept. 2005.

X. Gao, M. Laurenzano, B. Simon, and A. Snavely, *"Reducing Overheads for Acquiring Dynamic Traces,"* International Symposium on Workload Characterization (ISWC05), Austin, Texas, Sept. 2005.

R. Garnett, J. Billen, T. Wangler, P. Ostroumov, J. Qiang, R. Ryne, R. York, K. Crandall, *"Advanced Beam-Dynamics Simulation Tools for RIA,"* Proc. PAC2005, Knoxville, Tenn., May 2005.

C. Gatti-Bono, P. Colella, *"An anelastic all-speed projection method for gravitationally stratified flows,"* Journal of Computational Physics, in press.

L. Ge, L.-Q. Lee, Z. Li, C.-K. Ng, G. Schussman, L. Xiao and K. Ko, *"Advanced Eigensolver For Electromagnetic Modeling Of Accelerator Cavities,"* The 15th Conference on the Computation of Electromagnetic Fields, Shenyang, China, June 2005.

L. Ge, L.-Q. Lee, Z. Li, C.-K. Ng, K. Ko, E. Seol, A. C. Bauer and M. Shephard, *"Adaptive Mesh Refinement In Accelerator Cavity Design,"* SIAM Conference on Computational Science & Engineering, Orlando, Fla., Feb. 2005.

C. G. R. Geddes, C. Toth, J. van Tilborg, E. Esarey, C. B. Schroeder, D. Bruhwiler, C. Nieter, J. Cary, and W. P. Leemans, *"Production of high quality electron bunches by dephasing and beam loading in channeled and unchanneled laser plasma accelerators,"* Physics of Plasmas, **12**, 5, p. 56709, May 2005.

S. J. Ghan, and T. Shippert, *"Load balancing and scalability of a subgrid orography scheme in a global climate model,"* International Journal of High Performance Computer Applications., **19**, 237, 2005.

J. Glimm, X. L. Li, Z. L. Xu, *"Front tracking algorithm using adaptively refined meshes,"* Proc. of the 2003 Chicago Workshop on Adaptive Mesh Refinement Methods, Lecture Notes in Computational Science and Engineering, **41**, 83-90, 2005.

M. S. Gordon and M. W. Schmidt, *"Advances in Electronic Structure Theory: GAMESS a Decade Later,"* Theory and Applications of Computational Chemistry, Ch. 41, C. E. Dykstra, G. Frenking, K. S. Kim, G. E. Scuseria, Eds., Elsevier, 2005.

S. Gottlieb, et al., *"Onium masses with three flavors of dynamical quarks,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 203, 2005.

D. A. Goussis and M. Valorani, *"An efficient iterative algorithm for the approximation of the fast and slow dynamics of stiff systems,"* Journal of Computational Physics, **214**, 316, 2006.

D. A. Goussis, and M. Valorani, F. Creta and H. N. Najm, *"Reactive and Reactive/Diffusive Time Scales in Stiff Reaction-Diffusion Systems,"* Prog. in Computational Fluid Dynamics, **5**(6):316-326, Sept. 2005.

A. Gray, et al. (The HPQCD Collaboration), *"The B meson decay constant from unquenched lattice QCD,"* Physical Review Letters **95**, 212001, 2005.

A. Gray, et al. (The HPQCD Collaboration), *"The Upsilon spectrum and m(b) from full lattice QCD,"* Physical Review D, **72**, 094507, 2005.

A. Gray, et al. (The HPQCD Collaboration), *"B Leptonic Decays and B_B Mixing with 2+1 Flavors of Dynamical Quarks,"* Nuclear Physics (Proc. Suppl.) **140**, 446, 2005.

J. F. Grcar, M. S. Day, and J. B. Bell, *"A Taxonomy of Integral Reaction Path Analysis,"* Combust. Theory Modelling, to appear.

C. M. Greenfield, *"Advanced Tokamak Research at the DIII-D National Fusion Facility in Support of ITER,"* Proceedings of SciDAC 2005, Journal of Physics: Conference Series, Institute of Physics, San Francisco, Calif., June 2005.

M. Greenwald, D. P. Schissel, J. R. Burruss, T. Fredian, J. Lister and J. Stillerman, *"Visions for Data Management and Remote Collaboration on ITER,"* Proc. of ICALEPCS05, 2005.

E. Gulez, et al. (The HPQCD Collaboration), *"B Semileptonic Decays with 2+1 Dynamical Quark Flavors,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 220, 2005.

O. D. Gurcan, P. H. Diamond, T. S. Hahm and Z. Lin, *"Dynamics of Turbulence Spreading in Magnetically Confined Plasmas,"* Physics of Plasmas, **12**, 032303, 2005.

A. T. Hagler, et al. (The LHPC Collaboration), *"Helicity dependent and independent generalized parton distributions of the nucleon in lattice QCD,"* European Physics Journal, A24S1, **29**, 2005.

T. S. Hahm, P. H. Diamond, Z. Lin, G. Rewoldt, O. Gurcan, and S. Ethier, *"On the Dynamics of Edge-Core Coupling,"* Physics of Plasmas, **12**, 090903, 2005.

K. Hashimoto, T. Izubuchi and J. Noaki, *"The static quark potential in 2+1 flavour domain wall QCD from QCDOC,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 093, 2005.

J. C. Hayes, S. W. Bruenn, *"Toward 2-D and 3-D simulations of core-collapse supernovae with magnetic fields,"* Journal of Physics Conference Series, **16**, 395-399, 2005.

Y. He and C. Ding, *"Coupling Multi-Component Models with MPH on Distributed Memory Computer Architectures,"* International Journal of High Performance Computing Applications, **19**, 3, p. 329, 2005.

M. Head-Gordon, G. J. O. Beran, A. Sodt and Y. Jung, *"Fast electronic structure methods for strongly correlated molecular systems,"* Journal of Physics: Conf. Ser. **16**, 233-242, 2005.

A. Heger, E. Kolbe, W. C. Haxton, K. Langanke, G. Martinez-Pinedo and S. E. Woosley, *"Neutrino nucleosynthesis,"* Physics Letters B, **606**, 258-264, Jan. 2005.

A. Heger, S. E. Woosley and H. C. Spruit, *"Presupernova Evolution of Differentially Rotating Massive Stars Including Magnetic Fields,"* ApJ, **62**6:350-363, June 2005.

J. J. Heys, C. G. DeGroff, T. Manteuffel, and S. McCormick, *"First-order system least squares (FOSLS) for modeling blood flow,"* Med. Eng. Phys., to appear.

A. C. Hindmarsh, P. N. Brown, K. E. Grant, S. L. Lee, R. Serban, D. E. Shumaker, and C. S. Woodward, *"SUNDIALS: Suite of Nonlinear and Differential/Algebraic Equation Solvers,"* ACM Transactions on Mathematical Software, **31**(3), p. 363-396, 2005.

W. R. Hix, O. E. B. Messer, A. Mezzacappa, M. Liebendoerfer, D. J. Dean, K. Langanke, J. Sampaio, G. Martinez-Pinedo, *"Terascale input physics: the role of nuclear electron capture in core collapse supernovae,"* Journal of Physics Conference Series, **16**, 400-404, 2005.

W. R. Hix, B. S. Meyer, *"Thermonuclear Kinetics in Astrophysics,"* Nuclear Physics A, in press, Sept. 2005.

F. M. Hoffman, W. W. Hargrove, D. J. Erickson III and W. Oglesby, *"Using clustered climate regimes to analyze and compare predictions from fully coupled general circulation models,"* Earth Interactions, **9**, 1, 2005.

F. M. Hoffman, M. Vertenstein, H. Kitabata, and J. B. White III. *"Vectorizing the Community Land Model (CLM),"* International Journal of High Performance Computing Applications, **19**(3), 247, Aug. 2005.

F. M. Hoffman, W. W. Hargrove, D. J. Erickson, and R. J. Oglesby, *"Using Clustered Climate Regimes to Analyze and Compare Predictions from Fully Coupled General Circulation Models,"* Earth Interactions, **9**(10), 1-27, Aug. 2005.

I. Hofmann, G. Franchetti, A. U. Luccio, M. Giovannozzi, E. Métral, J. F. Amundson, P. Spentzouris, S. Machida, J. Qiang, R. Ryne, S. M. Cousineau, J. A. Holmes, F. Jones, *"Benchmarking of Simulation Codes Based on the Montague Resonance in the CERN-PS,"* Proc. PAC2005, Knoxville, Tenn., May 2005.

M. J. Hogan, C. D. Barnes, C. E. Clayton, F. J. Decker, S. Deng, P. Emma, C. Huang, R. H. Iverson, D. K. Johnson, C. Joshi, T. Katsouleas, P. Krejcik, W. Lu, K. A. Marsh, W. B. Mori, P. Muggli, C. L. O'Connell, E. Oz, R. H. Siemann and D. Walz, *"Multi-GeV Energy Gain in a Plasma-Wakefield Accelerator,"* Physical Review Letters **95**, 054802, 2005.

J. Hollingsworth, A. Snavely, S. Sbaraglia, and K. Ekanadham, *"EMPS: An Environment for Memory Performance Studies,"* IPDPS 2005, Next Generation Software Workshop, to appear.

D. J. Holmgren, *"PC clusters for lattice QCD,"* Nuclear Physics (Proc. Suppl.) **140**, 183, 2005.

D. J. Holmgren, *"U.S. Lattice Clusters and the USQCD Project,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 105, 2005.

C. Homescu, L. Petzold, and R. Serban, *"Error estimation for reduced order models of dynamical systems,"* SIAM Journal on Numerical Analysis, **43**, 1693, 2005.

E. B. Hooper, R. A. Kopriva, B. I. Cohen, D. N. Hill, H. S. McLean, R. D. Wood, S. Woodruff and C. R. Sovinec, *"A magnetic meconnection event in a driven spheromak,"* Physics of Plasmas **12**, 092503, 2005.

I. Horvath, et al., *"Inherently Global Nature of Topological Charge Fluctuations in QCD,"* Physics Letters B, **612**, 21, 2005.

I. Horvath, et al., *"The Negativity of the Overlap-Based Topological Charge Density Correlator in Pure-Glue QCD and the Non-Integrable Nature of its Contact Part,"* Physics Letters B, **617**, 49, 2005.

M. Huang, and B. Bode, "*A Performance Comparison of Tree and Ring Topologies in Distributed Systems,"* Parallel and Distributed Scientific and Engineering Computing PDSEC-05, Denver, Colo., April 2005.

A. L. Hungerford, C. L. Fryer, and G. M. Rockefeller, *"Gamma-Rays from Single Lobe Supernova Explosions,"* ArXiv Astrophysics e-prints, July 2005.

F.-N. Hwang, and X.-C. Cai, *"Parallel fully coupled Schwarz preconditioners for saddle point problems,"* Electronic Transactions on Numerical Analysis, 2005.

F.-N. Hwang, and X.-C. Cai, *"A parallel nonlinear additive Schwarz preconditioned inexact Newton algorithm for incompressible Navier-Stokes equations,"* Journal of Computational Physics, **204**, p. 666-691, 2005.

F.-N. Hwang, and X.-C. Cai, *"A combined linear and nonlinear preconditioning technique for incompressible Navier-Stokes equations,"* J. Dongarra, K. Madsen, and J. Wasniewski, eds., Lecture Notes in Computer Science, **3732**, p. 313-322, Springer-Verlag, 2005.

E. Ipek, B. R. de Supinski, M. Schulz and S. A. McKee, *"An Approach to Performance Prediction for Parallel Applications,"* Euro-Par 2005, Lisbon, Portugal, Sept. 2005.

R. Jacob, J. Larson, and E. Ong, *"MxN Communication and Parallel Interpolation in CCSM3 Using the Model Coupling Toolkit,"* International Journal of High Performance Computational Applications, **19**(3), 293, 2005.

E. F. Jaeger, *"Self-consistent full-wave and Fokker-Planck calculations for ion cyclotron heating in non-Maxwellian plasmas,"* Bull. American Physics Society **50**, 257, 2005.

E. F. Jaeger, L. A. Berry, R. W. Harvey, et al., *"Self-Consistent Full-Wave / Fokker-Planck Calculations for Ion Cyclotron Heating in non-Maxwellian Plasmas,"* Radio Frequency Power in Plasmas, Proc. 16th Topical Conf., Park City, Utah, 2005.

S. C. Jardin, J. A. Breslau, *"Implicit solution of the four-field extended-magnetohydrodynamic equations using high-order high-continuity finite elements,"* Physics of Plasmas **12**, 10, 2005.

J.E. Jones and B. Lee, *"A Multigrid Method for Variable Coefficient Maxwell's Equations,"* SIAM Journal on Scientific Computing, **27**, 168, 2006.

P. W. Jones, P. H. Worley, Y. Yoshida, J. B. White III and J. Levesque, *"Practical performance portability in the Parallel Ocean Program (POP),"* Concurrency Computation-Practice Experiment & Experience, **17**, 1317, 2005.

C. Jung, *"Thermodynamics using p4-improved staggered fermion action on QCDOC,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), **150**, 2005.

A. Juodagalvis, D. J. Dean, *"Gamow-Teller GT+ distributions in nuclei with mass A = 90-97,"* Physical Review C, **72**, 024306, 2005.

A. Juodagalvis, K. Langanke, G. Martinez-Pinedo, W. R. Hix, D. J. Dean, J. M. Sampaio, *"Neutral-current neutrino-nucleus cross sections for A~50-65 nuclei,"* Nuclear Physics A, **747**, 87-108, 2005.

D. J. Kerbyson and P. W. Jones, *"A Performance Model of the Parallel Ocean Program,"* International Journal of High Performance Computing Applications, **19**, 261, 2005.

C. C. Kim, C. R. Sovinec, S. E. Parker and the NIMROD Team, *"Hybrid kinetic-MHD simulations in general geometry,"* Computer Physics Communications **164**, 1-3, 448, 2005.

S. Klasky, *"Data Management on the Fusion Computational Pipeline,"* invited talk, SciDAC Conference, San Francisco, Calif., June 2005.

A. Klawonn, O. Rheinbach and O. Widlund, *"Some Computational Results for Dual-Primal FETI Methods for Elliptic Problems in 3D,"* Proc. of the 15th International Symposium on Domain Decomposition Methods, Berlin, Germany, July 2003.

A. Klawonn and O. Widlund, *"Selecting Constraints in Dual-Primal FETI Methods for Elasticity in Three Dimensions,"* Proc. of the 15th International Symposium on Domain Decomposition Methods, Berlin, Germany, July 2003.

K. Ko, N. Folwell, L. Ge, A. Guetz, L.-Q. Lee, Z. Li, C.-K. Ng, E. Prudencio, G. Schussman, R. Uplenchwar and L. Xiao, *"Advances in Electromagnetic Modeling through High Performance Computing,"* Proc. of 12th International Workshop on RF Superconductivity (SRF 2005), Cornell, New York, July 2005.

K. Ko, N. Folwell, L. Ge, A. Guetz, V. Ivanov, A. Kabel, M. Kowalski, L. Lee, Z. Li, C. Ng, E. Prudencio, G. Schussman, R. Uplenchwar, L. Xiao, E. Ng, W. Gao, X. Li, C. Yang, P. Husbands, A. Pinar, D. Bailey, D. Gunter, L. Diachin, D. Brown, D. Quinlan, R. Vuduc, P. Knupp, K. Devine, J. Kraftcheck, O. Ghattas, V. Akcelik, D. Keyes, M. Shephard, E. Seol, A. Brewer, G. Golub, K. Ma, H. Yu, Z. Bai, B. Liao, T. Tautges and H. Kim, *"Impact of SciDAC on accelerator projects across the Office of Science through electromagnetic modeling,"* Proc. of SciDAC 2005 meeting, San Francisco, Calif., June 2005.

S. Kronfeld, et al. (The Fermilab Lattice and MILC Collaborations), *"Predictions from Lattice QCD,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 206, 2005.

S. E. Kruger, C. R. Sovinec, D. D. Schnack and E. D. Held, *"Free-boundary simulations of DIII-D plasmas with the NIMROD code,"* Computer Physics Communications **164**, 1-3, 34, 2005.

S. E. Kruger, D. D. Schnack and C. R. Sovinec, *"Dynamics of the major disruption of a DIII-D plasma,"* Physics of Plasmas **12**, 056113, 2005.

M. Kuhlen, S. E. Woosley and G. A. Glatzmaier, *"Carbon Ignition in Type Ia Supernovae: II. A Three-Dimensional Numerical Model,"* ApJ **640**, 407, 2006.

J.-F. Lamarque, J. T. Kiehl, P. G. Hess, W. D. Collins, L. K. Emmons, P. Ginoux, C. Luo and X. X. Tie, *"Response of a coupled chemistry-climate model to changes in aerosol emissions: Global impact on the hydrological cycle and the tropospheric burdens of OH, ozone and NOx,"* Geophysical Research Letter, **32**, 16, L16809, 2005.

C.-L. Lappen and D. A. Randall, *"Using idealized coherent structures to parameterize momentum fluxes in a PBL mass-flux model,"* Journal of Atmospheric Sciences, **62**, 2829, 2005.

J. Larson, R. Jacob and E. Ong, *"The Model Coupling Toolkit: A New Fortran90 Toolkit for Building Multi-Physics Parallel Coupled Models,"* International Journal of High Performance Computing Applications, **19**(3), 277-292, 2005.

M. Laurenzano, B. Simon, A. Snavely and M. Gunn, *"Low Cost Trace-driven Memory Simulation Using SimPoint,"* Workshop on Binary Instrumentation and Applications, St. Louis, Mo., Sept. 2005.

I. Lee, P. Raghavan, and E. G. Ng, *"Effective Preconditioning Through Ordering Interleaved with Incomplete Factorization,"* SIAM J. Matrix Anal. Appls., **27**, 106, 2006.

J. C. Lee, H. N. Najm, S. Lefantzi, J. Ray, M. Frenklach, M. Valorani and D. A. Goussis, *"On chain branching and its role in homogeneous ignition and premixed flame propagation,"* Computational Fluid and Solid Mechanics 2005, K. J. Bathe, ed., p. 717, Elsevier, 2005.

L.-Q. Lee, Z. Bai, W. Gao, L. Ge, Z. Li, C.-K. Ng, C. Yang, E. Ng and K. Ko, *"Nonlinear Eigenvalue Problem in Accelerator Cavity Design,"* SIAM Annual Meeting, New Orleans, La., July 2005.

L.-Q. Lee, Z. Bai, W. Gao, L. Ge, P. Husbands, M. Kowalski, X. Li, Z. Li, C.-K. Ng, C. Yang, E. Ng and K. Ko, *"Modeling Rf Cavities With External*

Coupling," SIAM Conference on Computational Science & Engineering, Orlando, Fla., Feb. 2005.

L.-Q. Lee, L. Ge, Z. Li, C. Ng, G. Schussman, K. Ko, E. Ng, W. Gao, P. Husbands, X. Li, C. Yang, V. Akcelik, O. Ghattas, D. Keyes, T. Tautges, H. Kim, J. Craftcheck, P. Knupp, L. Freitag Diachin, K.-L. Ma, Z. Bai and G. Golub, *"Achievements in ISICs/SAPP collaborations for electromagnetic modeling of accelerators,"* Proc. of SciDAC 2005 meeting, San Francisco, Calif., June 2005.

W. P. Leemans, E. Esarey, J. van Tilborg, P. A. Michel, C. B. Schroeder, C. Toth, C. G. R. Geddes and B. A. Shadwick, *"Radiation from laser accelerated electron bunches: coherent terahertz and femtosecond x-rays,"* IEEE Trans. Plasma Sci., **33**, 1, 0093-3813, Feb. 2005.

S. Lefantzi, J. Ray, C. A. Kennedy and H. N. Najm, *"A Component-based Toolkit for Reacting Flows with Higher Order Spatial Discretizations on Structured Adaptively Refined Meshes,"* Prog. in Computational Fluid Dynamics, **5**(6), 298-315, Sept. 2005.

J. L. V. Lewandowski, *"Low-noise collision operators for particle-in-cell simulations,"* Physics of Plasmas, **12**, 052322, 2005.

J. L. V. Lewandowski, *"Global particle-in-cell simulations of microturbulence with kinetic electrons,"* invited talk, APS/DPP meeting, Denver, Colo., 2005.

H. Li, and M. S. Gordon, *"Gradients of the Exchange-Repulsion Energy in the Effective Fragment Potential Method,"* Theoretical Chemistry Accounts, in press.

K. Li, et al., *"Dynamic Scalable Visualization for Collaborative Scientific Applications,"* Proceedings of the Next Generation Software Workshop, Denver Colo., April 2005.

X. Li, M. S. Shepard, M. W., Beall, *"3-D Anisotropic Mesh Adaptation by Mesh Modifications,"* Computer Methods in Applied Mechanics and Engineering, **194**(48-49), p. 4915-4950, 2005.

X. S. Li, *"An Overview of SuperLU: Algorithms, Implementation, and User Interface,"* ACM Trans. on Math. Software, **31**, 3, 2005.

X. S. Li, W. Gao, P. J. R. Husbands, C. Yang and E. G. Ng, *"The Roles of Sparse Direct Methods in Large-Scale Simulations,"* Proc. of SciDAC 2005 meeting, San Francisco, Calif., June 2005.

Z. Li, A. Kabel, L. Ge, R. Lee, C.-K. Ng, G. Schussman, L. Xiao and K. Ko, *"Electromagnetic Modeling For The ILC,"* International Linear Collider Physics and Detector Workshop and 2nd ILC accelerator Workshop, Snowmass, Colo., Aug. 2005.

M. Liebendoerfer, M. Rampp, H.-T. Janka, A. Mezzacappa, "*Supernova Simulations with Boltzmann Neutrino Transport: A Comparison of Methods,"* Astrophysical Journal Letters, **620**, 840-860, 2005.

H.-W. Lin and N. H. Christ, *"Non-perturbatively determined relativistic heavy quark action,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 225, 2005.

M.-F. Lin, *"Probing the chiral limit ofMpi and fpi _in 2+1 flavor QCD with domain wall fermions from QCDOC,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), **94**, 2005.

Y. Lin, S. Wukitch, A. Parisot, J. C. Wright, N. Basse, P. Bonoli, E. Edlund, L. Lin, M. Porkolab, G. Schilling and P. Phillips, *"Observation and modeling of ion cyclotron range of frequencies waves in the mode conversion region of Alcator C-Mod,"* Plasma Phys. and Control. Fusion **47**, 1207, 2005.

Y. Lin, X. Wang, Z. Lin, and L. Chen, *"A Gyrokinetic Electron and Fully Kinetic Ion Plasma Simulation Model,"* Plasma Phys. Contr. Fusion **47**, 657, 2005.

Z. Lin, L. Chen, and F. Zonca, *"Role of Nonlinear Toroidal Coupling in Electron Temperature Gradient Turbulence,"* Physics of Plasmas, **12**, 056125, 2005.

D.-J. Liu and J. W. Evans, *"From Atomic Scale Ordering to Mesoscale Spatial Patterns in Surface Reactions: A Heterogeneous Coupled Lattice-Gas (HCLG) Simulation Approach,"* SIAM Multiscale Modeling and Simulation, **4**, 424, 2005.

K. F. Liu and N. Mathur, *"A Review of Pentaquark Calculations on the Lattice,"* Proc. of 2005 Int. Conf. on QCD and Hadron Physics, 2005.

X. Luo, L. Yin, M. S. Shephard, R. M. O'Bara, M. W. Beall, *"An automatic adaptive directional variable p-version method for 3-D curved domains,"* Proc. 8th US Nat. Congress on Comp. Mech., 2005.

E. Lusk, N. Desai, R. Bradshaw, A. Lusk and R. Butler, *"An Interoperability Approach to System Software, Tools and Libraries for Clusters,"* International Journal of High Performance Computing Applications (to appear 2006).

K. L. Ma, E. B. Lum, H. Yu, H. Akiba, M. Y. Huang, M.-Y. Huang, Y. Wang and G. Schussman, *"Scientific Discovery through Advanced Visualization,"* Journal of Physics, **16**, DOE SciDAC 2005 Conference, San Francisco, Calif., June 2005.

Q. Mason et al. (The HPQCD Collaboration), *"Accurate determinations of alpha(s) from realistic lattice QCD,"* Physical Review Letters **95**, 052002, 2005.

T. Manteuffel, S. McCormick, J. Ruge and J. G. Schmidt, *"First-order system LL* (FOSLL*) for general scalar elliptic problems in the plane,"* SIAM Journal on Numerical Analysis, **43**, 209, 2005.

T. Manteuffel, S. McCormick, O. Röhrle and J. Ruge, *"Projection multilevel methods for quasilinear elliptic partial differential equations: numerical results,"* SIAM Journal on Numerical Analysis, **44**, 120, 2006.

T. Manteuffel, S. McCormick and O. Röhrle, *"Projection multilevel methods for quasilinear elliptic partial differential equations: theoretical results,"* SIAM Journal on Numerical Analysis, **44**, 139, 2006.

J. Marathe, F. Mueller and B. R. de Supinski, *"A Hybrid Hardware/Software Approach to Efficiently Determine Cache Coherence Bottlenecks,"* Proc. of the International Conference on Supercomputing, Heidelberg, Germany, June 2005.

D. F. Martin, P. Colella, M. Anghel, F. Alexander, *"Adaptive mesh refinement for multiscale nonequilibrium physics,"* Computers in Science and Engineering, **7**, 3, p. 24-31, 2005.

N. Mathur, et al., *"Roper Resonance and S11(1535) from Lattice QCD,"* Physics Letters B, **605**, 137, 2005.

S. McCormick, *"Projection multilevel methods for quasilinear elliptic partial differential equations: V-cycle theory,"* SIAM J. Mult. Modeling Sim., **4**, 133, 2006.

P. McCorquodale, P. Colella, G. Balls, S. B. Baden, *"A scalable parallel Poisson solver with infinite domain boundary conditions,"* Proc. of the 7th Workshop on High Performance Scientific and Engineering Computing, Oslo, Norway, June 2005.

D. M. Medvedev, E. M. Goldfield and S. K. Gray, *"An OpenMP/MPI Approach to the Parallelization of Iterative Four-Atom Quantum Mechanics,"* Computer Physics Comm. **166**, 94-108, 2005.

D. M. Medvedev, S. K. Gray, A. F. Wagner, M. Minkoff and R. Shepard, *"Advanced Software for the Calculation of Thermochemistry, Kinetics, and Dynamics,"* Journal of Physics: Conference Series **16**, 247-251, 2005.

J. E. Menard, R. E. Bell, E. D. Fredrickson, W. Park, et al., *"Internal kink mode dynamics in high-beta NSTX plasmas,"* Nuclear Fusion **45** (7), 539-556, 2005.

A. Mezzacappa, *"Ascertaining the Road Ahead,"* Annual Review of Nuclear and Particle Science, **55**, 467-515, 2005.

B. Mohr, A. Khnal, M.-A. Hermanns, F. Wolf, *"Performance Analysis of One-sided Communication Mechanisms," Mini-Symposium "Tools Support for Parallel Programming,"* Proc. of Parallel Computing (ParCo), Malaga, Spain, Sept. 2005.

S. Moore, F. Wolf, J. Dongarra, S. Shende, A. Malony, B. Mohr, *"A Scalable Approach to MPI Application Performance Analysis,"* Proc. of the 12th European Parallel Virtual Machine and Message Passing Interface Conference, Sept. 2005.

S. Moore, F. Wolf, J. Dongarra, B. Mohr, *"Improving Time to Solution with Automated Performance Analysis,"* Second Workshop on Productivity and Performance in High-End Computing, 11th International Symposium on High Performance Computer Architecture (HPCA-2005), San Francisco, Calif., Feb. 2005.

J. Mueller, O. Sahni, K. E. Jansen, M. S. Shephard, *"An anisotropic mesh adaption procedure for pulsatile blood flow simulation,"* Proc. 8th US Nat. Congress on Comp. Mech., 2005.

J. Mueller, O. Sahni, K. E. Jansen, M. S. Shephard, C. A. Taylor, *"A tool for the efficient FE-simulation of cardio-vascular flow,"* Proc. 2nd NAFEMS CFD Seminar: Simulation of Complex Flows (CFD), April 2005.

B. Mustapha, V. N. Aseev, P. Ostroumov, J. Qiang, R. Ryne, *"RIA Beam Dynamics: Comparing TRACK to IMPACT,"* Proc. of Particle Accelerator Conference (PAC 05), Knoxville, Tenn., May 2005.

J. R. Myra, D. A. D'Ippolito, D. A. Russell, L. A. Berry, E. F. Jaeger and M. D. Carter, *"Nonlinear IRCR-Plasma Interactions,"* Radio Frequency Power in Plasmas, Proc. 16th Topical Conf., Park City, Utah, 2005.

H. N. Najm, J. C. Lee, M. Valorani, D. A. Goussis and M. Frenklach, *"Adaptive chemical model reduction,"* Journal of Physics: Conference Series, **16**, 101-106, June 2005.

D. Narayan, *"Bcfg2: A Pay As You Go Approach to Configuration Complexity,"* Proc. of the 2005 Australian UNIX Users Group, Sydney, Australia, Oct. 2005.

D. Narayan, E. Lusk and R. Bradshaw, *"{MPISH2}: Unix integration for {MPI} programs,"* Proc, of EuroPVM-MPI 2005, Sept. 2005.

H. Nassar, M. Paul, I. Ahmand, J. Ben-Dov, J. Caggiano, S. Ghelberg, S. Goriely, J. P. Greene, M. Hass, A. Heger, A. Heinz, D. J. Henderson, R. V. F. Janssens, C. L. Jiang, Y. Kashiv, B. S. Nara Singh, A. Ofan, R. C. Pardo, T. Pennington, K. E. Rehm, G. Savard, R. Scott and R. Vondrasek, *"The 40Ca(_,_)44Ti reaction in the energy regime of supernova nucleosynthesis,"* Physical Review Letters, **96**, 041102, 2006.

Y. Nishimura, Z. Lin, J. L. V. Lewandowski and S. Ethier, *"A Finite Element Poisson Solver for Global Gyrokinetic Particle Simulations in a Global Field Aligned Mesh,"* Journal of Computation & Physics, **214**, 657, 2006.

B. Norris, L. McInnes, and I. Veljkovic, *"Computational quality of service in parallel CFD,"* Proc. of the 17th International Conference on Parallel Computational Fluid Dynamics, University of Maryland, College Park, Md., May 2005.

M. Nuggehally, M. Picu, C. Shephard, M. S. Shephard, *"Adaptive model selection procedure in multiscale problems,"* Proc. 8th US Nat. Congress on Comp. Mech., 2005.

M. Okamoto, et al. (The Fermilab Lattice, HPQCD and MILC Collaborations), *"Semileptonic D _ _/K and B _ _ /D decays in 2+1 flavor lattice QCD,"* Nuclear Physics B (Proc. Suppl.) **140**, 461, 2005.

L. Oliker, J. Carter, M. Wehner, A. Canning, S. Ethier, A. Mirin, G. Bala, D. Parks, P. Worley, S. Kitawaki and Y. Tsuda, *"Leading Computational Methods on Scalar and Vector HEC Platforms,"* Proc. of the ACM/IEEE SC05 conference, Seattle, Wash., Nov. 2005.

O. O. Oluwole and W. H. Green, *"Rigorous Error Control in Reacting Flow Simulations Using Reduced Chemistry Models,"* Computational Fluid and Solid Mechanics: Proceedings of the Third MIT Conference on Computational Fluid and Solid Mechanics, ed. by K. J. Bathe, Elsevier, 2005.

C. D. Ott, S. Ou, J. E. Tohline and A. Burrows, *"One-armed Spiral Instability in a Low-T/\W\ Postbounce Supernova Core,"* ApJ. Letters, **625**:L119-L122, June 2005.

C. Ozen, D. J. Dean, *"Shell Model Monte Carlo method in the pn-formalism and applications to the Zr and Mo isotopes,"* ArXiv Nuclear Theory e-prints, Aug. 2005.

J. E. Penner, M. Herzog, C. Jablonowski, B. van Leer, R. C. Oehmke, Q. F. Stout and K. G. Powell, *"Development of an atmospheric climate model with self-adapting grid and physics,"* Journal of Physics: Conference Series, **16**, 353, 2005.

P. Petreczky, K. Petrov, D. Teaney and A. Velytsky, *"Heavy quark diffusion and lattice correlators,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 185, 2005.

K. Petrov, A. Jakovac, P. Petreczky and A. Velytsky, *"Bottomonia correlators and spectral functions at zero and finite temperature,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 153, 2005.

J. Petrovic, N. Langer, S.-C. Yoon and A. Heger, *"Which massive stars are gamma-ray burst progenitors?"* Astronomy & Astrophysics, **435**:247-259, May 2005.

L. R. Petzold, Y. Cao, S. Li and R. Serban, *"Sensitivity Analysis of Differential-Algebraic Equations and Partial Differential Equations,"* Proc. of the Chemical Process Control Conference, Lake Louise, Alberta, Canada, Jan. 2006.

J. Pjesivac-Grbovic, T. Angskun, G. Bosilca, G. Fagg, E. Gabriel, J. Dongarra, *"Performance Analysis of MPI Collective Operations,"* 4th International Workshop on Performance Modeling, Evaluation, and Optmization of Parallel and Distributed Systems (PMEO-PDS 2005), Denver, Colo., April 2005.

A. Pochinsky, *"Domain Wall Fermion Inverter on Pentium 4,"* Nuclear Physics B (Proc. Suppl.) **140**, 859, 2005.

E. Prudencio, R. Byrd, and X.-C. Cai, *"Parallel full space SQP Lagrange-Newton-*

Krylov-Schwarz algorithms for PDE-constrained optimization problems," SIAM Journal of Scientific Computing, **27**, 130, 2006.

J. Pruet, S. E. Woosley, R. Buras, H.-T. Janka and R. D. Hoffman, *"Nucleosynthesis in the Hot Convective Bubble in Core-Collapse Supernovae,"* ApJ, **623**:325-336, April 2005.

J. Qiang, *"Terascale Beam-Beam Simulations for Tevatron, RHIC and LHC,"* Proc. PAC2005, Knoxville, Tenn., May 2005.

J. Qiang, M. A. Furman, R. D. Ryne, W. Fischer, K. Ohmi, *"Recent advaces of strong-strong beam-beam simulation,"* Nuclear Instruments & Methods in Physics Research A, **558**, 351, 2006.

J. Qiang, S. M. Lidia, R. Ryne, C. Limborg-Deprey, *"A 3D Parallel Beam Dynamics Code for Modeling High Brightness Beams in Photoinjectors,"* Proc. PAC2005, Knoxville, Tenn., May 2005.

J. Qiang, D. Leitner, D. Todd, *"A Parallel 3D Model for the Multi-Species Low Energy Beam Transport System of the RIA Prototype ECR Ion Source VENUS,"* Proc. PAC2005, Knoxville, Tenn., May 2005.

P. Raghavan, M. J. Irwin, L. C. McInnes and B. Norris, *"Adaptive software for scientific computing: Co-managing quality-performance-power tradeoffs,"* Proc. of the IEEE International Parallel & Distributed Processing Symposium 2005, IEEE Computer Society Press, 2005.

J. J. Ramos, *"Fluid formalism for collisionless magnetized plasmas,"* Physics of Plasmas **12**, 052102, 2005.

J. J. Ramos, "General expression of the gyro-viscous force," Physics of Plasmas **12**, 112301, 2005.

N. S. Rao, S. M. Carter, Q. Wu, W. R. Wing, M. Zhu, A. Mezzacappa, M. Veeraraghavan, J. M. Blondin, *"Networking for large-scale science: infrastructure, provisioning, transport and application mapping,"* Journal of Physics Conference Series, **16**, 541-545, 2005.

J. Ray, C. Kennedy, J. Steensland and H. Najm, *"Advanced algorithms for computations on block-structured adaptively refined meshes,"* Journal of Physics: Conference Series, **16**:113-118, June 2005.

D. A. Reed, C. Lu and C. L. Mendes, *"Reliability Challenges in Large Systems,"* Future Generation Computer Systems, **22**, 293,2006.

J. F. Remacle, S. S. Frazao, M. S. Shephard, M. S. Flaherty, *"An Adaptive Discretization of Shallow Water Equations based on Discontinuous Galerkin Methods,"* International Journal for Numerical Methods in Fluids, **62**(7), pp. 899-923, 2005.

J. F. Remacle, X. Li, M. S. Shephard, J. E. Flaherty, *"Anisotropic Adaptive Simulation of Transient Flows using Discontinuous Galerkin Methods,"* International Journal for Numerical Methods in Engineering, **62**, pp. 899-923, 2005.

D. B. Renner, et al. (The LHPC Collaboration), *"Hadronic physics with domain-wall valence and improved staggered sea quarks,"* Nuclear Physics. (Proc. Suppl.) **140**, 255, 2005.

G. Rewoldt, *"Particle-In-Cell simulations of electron transport,"* invited talk, SciDAC Conference, San Francisco, Calif., June 2005.

D. G. Richards, *"Lattice studies of baryons,"* Journal of Physics Conf. Ser. **9**, 238, 2005.

G. Rockefeller, C. L. Fryer, F. K. Baganoff and F. Melia, *"The X-ray Ridge Surrounding Sgr A* at the Galactic Center,"* ArXiv Astrophysics e-prints, June 2005.

G. Rockefeller, C. L. Fryer, and F. Melia, *"Spin-Induced Disk Precession in Sagittarius A*,"* ArXiv Astrophysics e-prints, July 2005.

F. K. Roepke, W. Hillebrandt, J. C. Niemeyer, and S. E. Woosley, *"Multi-spot ignition in type Ia supernova models,"* ArXiv Astrophysics e-prints, Oct. 2005.

T. M. Rogers and G. A. Glatzmaier, *"Penetrative Convection within the Anelastic Approximation,"* ApJ, **620**:432-441, Feb. 2005.

D. Rotem, K. Stockinger, and K. Wu, *"Optimizing candidate check costs for bitmap indices,"* Proc. of CIKM 2005, ACM Press, 2005.

D. Rotem, K. Stockinger, and K. Wu, *"Optimizing i/o costs of multi-dimensional queries using bitmap indices,"* in DEXA, Lecture Notes in Computer Science **3588**, p. 220. Springer-Verlag, 2005.

B. Ruscic, J. E. Boggs, A. Burcat, A. G. Csaszar, J. Demaison, R. Janosche, J. M. L. Martin, M. L. Morton, M. J. Rossi, J. F. Stanton, P. G. Szalay, P. R. Westmoreland, F. Zabel, T. Berces, *"IUPAC critical evaluation of thermochemical properties of selected radicals: Part I,"* Journal of Physical and Chemical Reference Data, **34**(2), 573-656, 2005.

B. Ruscic, R. E Pinzon, G. Von Laszewski, D. Kodeboyina, A. Burcat, D. Leahy, D. Montoya, A. F. Wagner, *"Active thermochemical tables: Thermochemistry for the 21st Century,"* Journal of Physics: Conference Series, **16**:561-570, 2005.

R. Ryne, D. Abell, A. Adelmann, J. Amundson, C. Bohn, J. Cary, P. Colella, D. Dechow, V. Decyk, A. Dragt, R. Gerber, S. Habib, D. Higdon, T. Katsouleas, K.-L. Ma, P. McCorquodale, D. Mihalcea, C. Mitchell, W. Mori, C. T. Mottershead, F. Neri, I. Pogorelov, J. Qiang, R. Samulyak, D. Serafini, J. Shalf, C. Siegerist, P. Spentzouris, P. Stoltz, B. Terzic, M. Venturini, P. Walstrom, *"SciDAC Advances and Applications in Computational Beam Dynamics,"* Proceeding of SciDAC 2005, June 26-30, San Francisco, Calif., June 2005.

M. J. Savage, *"Nuclear Physics and QCD,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 020, 2005.

E. Scannapieco, P. Madau, S. Woosley, A. Heger and A. Ferrara, *"The Detectability of Pair-Production Supernovae at $z < 6$,"* Astrophysical Journal, **633**, 1031, 2005.

D. P. Schissel, *"Advances in Remote Participation for Fusion Experiments,"* Proc. of the 21st IEEE/NPSS Symposium on Fusion Engineering, 2005.

D. P. Schissel, et al., *"The Collaborative Tokamak Control Room,"* The 5th IAEA Technical Meeting on Control, Data Acquisition, and Remote Participation for Fusion Research, 2005.

D. P. Schissel, *"Advances in the Real-Time Interpretation of Fusion Experiments,"* Proceedings of SciDAC 2005, Journal of Physics: Conference Series, Institute of Physics, San Francisco, Calif., June 2005.

D. P. Schissel, et al., *"Grid Computing and Collaboration Technology in Support of Fusion Energy Sciences,"* Physics of Plasmas **12**, 058104, 2005.

D. P. Schissel, et al., *"Advances in Remote Participation for Fusion Experiments,"* The 23rd Symposium on Fusion Technology, 2005.

W. J. Schroeder, M. S. Shephard, *"Computational Visualization,"* Encyclopedia of Computational Mechanics, E. Stein, R. DeBorst, T.J.R. Hughes, eds., Wiley, 2005.

K. Schuchardt, O. Oluwole, W. Pitz, L. A. Rahn, J. William, H. Green, D. Leahy, C. Pancerella, M. Sjöberg and J. Dec, *"New Approaches for Collaborative Sharing of Chemical Model Data and Analysis Tools,"* 2005 Joint Meeting of the US Sections of the Combustion Institute, 2005.

K. Schuchardt, O. Oluwole, W. Pitz, L. A. Rahn, J. William, H. Green, D. Leahy, C. Pancerella, M. Sjöberg, J. Dec, *"Development of the RIOT web service and information technologies to enable mechanism reduction for HCCI simulations,"* Journal of Physics: Conference Series, **16**:107-112, 2005.

M. Schulz, D. Ahn, A. Bernat, B. R. de Supinski, S. Ko, G. Lee and B. Rountree, *"Scalable Dynamic Binary Instrumentation for BlueGene/L,"* Workshop on Binary Instrumentation and Applications, Sept. 2005.

P. Schwartz, D. Adalsteinsson, P. Colella, A. P. Arkin, M. Onsum, *"Numerical computation of diffusion on a surface,"* Proc. Nat. Acad. Sci., **102**, p. 11151-11156, 2005.

P. Schwartz, M. Barad, P. Colella, T. J. Ligocki, *"A Cartesian grid embedded boundary method for the heat equation and Poisson's equation in three dimensions,"* Journal of Computational Physics **211**, p. 531-550, 2006.

E. S. Seol, M. S. Shephard, *"A Flexible Distributed Mesh Data Structure to Support Parallel Adaptive Analysis,"* Proc. 8th US Nat. Congress on Comp. Mech., 2005.

R. Serban and A. C. Hindmarsh, *"CVODES: the Sensitivity-Enabled ODE Solver in SUNDIALS,"* Proc. of the 5th International Conference on Multibody Systems, Nonlinear Dynamics and Control, Long Beach, Calif., Sept. 2005.

B. A. Shadwick, G. M. Tarkenton, E. Esarey and C. B. Schroeder, *"Fluid and Vlasov models of low temperature, collisionless laser-plasma interactions,"* Physics of Plasmas, **12**, 5, p. 56710-18, May 2005.

S. Shende, A. Malony, A. Morris, F. Wolf, *"Performance Profiling Overhead Compensation for MPI Programs,"* Proc. of the 12th European Parallel Virtual Machine and Message Passing Interface Conference, Sept. 2005.

M. S. Shephard, A. C. Bauer, E. S. Seol, J. Wa., *"Construction of Adaptive Simulation Loops,"* Proc. 8th US Nat. Congress on Comp. Mech., 2005.

M. S. Shephard, J. E. Flaherty, K. E. Jansen, X. Li, X. j. Luo, N. Chevaugeon, J. F. Remacle, M. W. Beall, R. M. O'Bara, *"Adaptive mesh generation for curved domains,"* Applied Numerical Mathematics, **53**(2-3) p. 251-271, 2005.

R. Shepard, M. Minkoff, and Y. Zhou, *"Software for Computing Eigenvalue Bounds for Iterative Subspace Methods,"* Computer Physics Comm. **170**, 109-114, 2005.

M. S. Shephard, E. Seol, J. Wan, A. C. Bauer, *"Component-based adaptive control procedures,"* Proc. from the Conference on Analysis, Modeling and Computation of PDE and Multiphase Flow, Kluwer Academic Press, 2005.

J. Shigemitsu, et al. (The HPQCD Collaboration), *"Semileptonic B Decays with Nf = 2+1 Dynamical Quarks,"* Nuclear Physics (Proc. Suppl.) **140**, 464, 2005.

J. N. Simone, et al. (The Fermilab Lattice, HPQCD and MILC Collaborations), *"Leptonic decay constants fDs and fD in three flavor lattice QCD,"* Nuclear Physics B (Proc. Suppl.) **140**, 443, 2005.

A. Socrates, O. Blaes, A. Hungerford, and C. L. Fryer, *"The Neutrino Bubble Instability: A Mechanism for Generating Pulsar Kicks,"* Astrophysical Journal, **632**:531-562, Oct. 2005.

C. R. Sovinec, and C. C. Kim, D. D. Schnack, A. Y. Pankin, S. E. Kruger, E. D. Held, D. P. Brennan, D. C. Barnes, X. S. Li, D. K. Kaushik, S. C. Jardin and the NIMROD Team, *"Nonlinear Magnetohydrodynamic (MHD) Simulations using High-Order Finite Elements,"* SciDAC 2005 meeting, Journal of Physics: Conference Series, **16**, p. 25-34, San Francisco, Calif., June 2005.

C. Stan, *"The mean meridional circulation: A new potential-vorticity, potential-temperature perspective,"* Ph.D. thesis, Colorado State University. 2005.

A. W. Steiner, M. Prakash, J. M. Lattimer, P. J. Ellis, *"Isospin asymmetry in nuclei and neutron stars,"* Physics Reports, **411**, 325-375, 2005.

K. Stockinger, J. Shalf, E. W. Bethel and K. Wu, *"Dex: Increasing the capability of scientific data analysis pipelines by using efficient bitmap indices to accelerate scientific visualization,"* Proc. of 2005 Scientific and Statistical Database Management Conference, p. 35, 2005.

K. Stockinger, J. Shalf, E. W. Bethel and K. Wu, *"Query-driven visualization of large data sets,"* IEEE Visualization 2005, Minneapolis, MN, Oct. 2005.

K. Stockinger, K. Wu, R. Brun and P. Canal, *"Bitmap indices for fast end-user physics analysis in Root,"* Nuclear Instruments and Methods in Physics Research Section A, **539**, 99, 2006.

K. Stockinger, K. Wu, S. Campbell, S. Lau, M. Fisk, E. Gavrilov, A. Kent, C. E. Davis, R. Olinger, R. Young, J. Prewett, P. Weber, T. P. Caudell, E. W. Bethel and S. Smith, *"Network traffic analysis with query driven visualization,"* Proc. of the ACM/IEEE SC05 conference, Seattle, Wash., Nov. 2005.

P. Strack and A. Burrows, *"Generalized Boltzmann formalism for oscillating neutrinos,"* Physics Rev. D, **71**(9), 093004, May 2005.

L. Sugiyama, W. Park, H. R. Strauss, G. Fu, J. Breslau, J. Chen and S. Klasky, *"Plasmas beyond MHD: two-fluids and symmetry breaking,"* Journal of Physics: Conference Series **16**, 54-58, 2005.

F. D. Swesty, E. S. Myra, *"Multigroup models of the convective epoch in core collapse supernovae,"* Journal of Physics Conference Series, **16**, 380-389, 2005.

S. Tamhankar, et al., *"Charmonium Spectrum from Quenched QCD with Overlap Fermions,"* Nuclear Physics B (Proc. Suppl.), **140**, 434, 2005.

T. A. Thompson, E. Quataert, and A. Burrows, *"Viscosity and Rotation in Core-Collapse Supernovae,"* Astrophysical Journal, **620**:861-877, Feb. 2005.

D. Trebotich, G. H. Miller, P. Colella, D. T. Graves, D. F. Martin, P. O. Schwartz, "*A tightly coupled particle-fluid model for DNA-laden flows in complex microscale geometries,"* Proc. of the Third MIT Conference on Computational Fluid and Solid Mechanics, June 2005.

D. Trebotich, P. Colella, G. H. Miller, *"A stable and convergent scheme for viscoelastic flow in contraction channels,"* J. Comput. Phys. **205**, p. 315-342, 2005.

D. Todd, D. Leitner, C. Lyneis, J. Qiang, D. Grote, *"Particle-in-Cell Simulations of the*

VENUS Ion Beam Transport System," Proc. PAC2005, Knoxville, Tenn., May 2005.

D. Toussaint and C. Davies (MILC and UKQCD Collaborations), *"The Ω_ and the strange quark mass,"* Nuclear Physics B (Proc. Suppl.), **140**, 234, 2005.

T. Tu, D. O'Hallaron, and O. Ghattas, *"Scalable parallel octree meshing for terascale applications,"* Proceedings of the ACM/IEEE SC05 conference, Seattle, Wash., November 2005.

R. Tweedie, *"Light meson masses and decay constants in a 2+1 flavour domain wall QCD,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 080, 2005.

F. Y. Tzeng and K. L. Ma, *"Intelligent Feature Extraction and Tracking for Large-Scale 4D Flow Simulations,"* Proc. of the ACM/IEEE SC05 conference, Seattle, Wash., Nov. 2005.

M. Valorani, F. Creta, D. A. Goussis, H. N. Najm, and J. C. Lee, *"Chemical kinetics mechanism simplification via CSP,"* Computational Fluid and Solid Mechanics 2005, K. J. Bathe, ed., p. 900, Elsevier, 2005.

M. Valorani, D. A. Goussis, F. F. Creta and H. N. Najm, *"Higher Order Corrections in the Approximation of Low Dimensional Manifolds and the Construction of Simplified Problems with the CSP Method,"* Journal of Computational Physics, **209**(2), 754-786, Nov. 2005.

J-L. Vay, P. Colella, P. McCorquodale, D. Serafini, V. Straalen, A. Friedman, D. P. Grote, J-C. Adam, A. Héron, *"Application of Adaptive Mesh Refinement to Particle-In-Cell Simulations of Plasmas and Beams,"* Workshop on Multiscale Processes in Fusion Plasmas, IPAM, Los Angeles, Calif., Jan. 2005.

J.-L. Vay, M. Furman, R. Cohen, A. Friedman, D. Grote, *"Initial self-consistent 3-D electron-cloud simulations of LHC beam with the code WARP+POSINST,"* Proc. PAC2005, Knoxville, Tenn., May 2005.

J. Vetter, B. R. de Supinski, J. May, L. Kissel and S. Vaidya, *"Evaluating High Performance Computers,"* in Concurrency: Practice and Experience, **17**, 1239, 2005.

J. S. Vetter, S. R. Alam, T. H. Dunigan, Jr., M. R. Fahey, P. C. Roth and P. H. Worley, *"Early Evaluation of the Cray XT3 at ORNL,"* Proc. of the 47th Cray User Group Conference, Albuquerque, NM, May 2005.

R. Vuduc, J. Demmel and K. Yelick, *"OSKI: A library of automatically tuned sparse matrix kernels,"* Proc. of SciDAC 2005, Journal of Physics: Conference Series, San Francisco, Calif., June 2005.

R. Vuduc, and H.-J. Moon, *"Fast sparse matrix-vector multiplication by exploiting variable block structure,"* Proc. of the International Conference on High-Performance Computing and Communications, Sorrento, Italy, Sept. 2005.

G. Wallace, et al., *"Tools and Applications for Large-Scale Display Walls,"* IEEE Computer Graphics & Applications, Special Issue on Large Displays, **25**, 24, July/Aug. 2005.

R. Walder, A. Burrows, C. D. Ott, E. Livne, I. Lichtenstadt and M. Jarrah, *"Anisotropies in the Neutrino Fluxes and Heating Profiles in Two-dimensional, Time-dependent, Multigroup Radiation Hydrodynamics Simulations of Rotating Core-Collapse Supernovae,"* Astrophysical Journal, **626**:317-332, June 2005.

W. Wan, Y. Chen, S. E. Parker, *"Gyrokinetic delta f simulation of the collisionless and semicollisional tearing mode instability,"* Physics of Plasmas **12**, 012311, 2005.

J. Wan, M. S. Shephard, *"Contact Surface Control in Forming Simulations,"* Proc. 8th US Nat. Congress on Comp. Mech., 2005.

W. X. Wang, *"Neoclassical and turbulent transport in shaped toroidal plasmas,"* invited talk, APS/DPP meeting, Denver, Colo., 2005.

J. Weinberg, M. O. MCracken, A. Snavely, and E. Strohmaier, *"Quantifying Locality in the Memory Access Patterns of HPC Applications,"* Proc. of the ACM/IEEE SC05 conference, Seattle, Wash., Nov. 2005.

V. Wheatley, D. I. Pullin and R. Samtaney, *"On the regular refraction of a MHD shock at a density interface,"* Journal of Fluid Mechanics, **522**, 179-214, 2005.

V. Wheatley, D. I. Pullin, and R. Samtaney, and R. Samtaney, *"Stability of an impulsively accelerated density interface in MHD,"* Physical Review Letters **95**, 12, 2005.

B. S. White, S. A. McKee, B. R. de Supinski, B. Miller, D. Quinlan and M. Schulz, *"Improving the Computational Intensity of Unstructured Mesh Applications,"* Proceedings of the International Conference on Supercomputing, Heidelberg, Germany, June 2005.

B. Willems, M. Henninger, T. Levin, N. Ivanova, V. Kalogera, K. McGhee, F. X. Timmes, and C. L. Fryer, *"Understanding Compact Object Formation and Natal Kicks. I. Calculation Methods and the Case of GRO J1655-40,"* Astrophysical Journal, **625**, 324-346, May 2005.

F. Wolf, A. Malony, S. Shende, A. Morris, *"Trace-Based Parallel Performance Overhead Compensation,"* Proc. of the International Conference on High Performance Computing and Communications (HPCC), Sorrento, Italy, Sept.2005.

S. E. Woosley and T. Janka, *"The Physics of Core-Collapse Supernovae,"* Nature Physics, **1**, 147, 2005.

P. H. Worley, S. Alam, T. H. Dunigan, Jr., M. R. Fahey and J. S. Vetter, *"Comparative Analysis of Interprocess Communication on the X1, XD1, and XT3,"* Proc. of the 47th Cray User Group Conference, Albuquerque, NM, May 2005.

P. H. Worley and J. B. Drake, *"Performance Portability in the Physical Parameterizations of the Community Atmospheric Model,"* International Journal for High Performance Computer Applications, **19**(3), p. 187, Aug. 2005.

J. C Wright, L. A. Berry, P. T. Bonoli, D. B. Batchelor, E. F. Jaeger, M. D. Carter, E. D'Azevedo, C. K. Phillips, H. Okuda, R. W. Harvey, D. N. Smithe, J. R. Myra, D. A. D'Ippolito, M. Brambilla and R. J. Dumont, *"Nonthermal particle and full-wave diffraction effects on heating and current drive in the ICRF and LHRF regimes,"* Nuclear Fusion **45**, 1411, 2005.

J. C. Wright, P. T. Bonoli, M. Brambilla, E. D'Azevedo, L. A. Berry, D. B. Batchelor, E. F. Jaeger, M. D. Carter, C. K. Phillips, H. Okuda, R. W. Harvey, J. R. Myra, D. D'Ippolito and D. N. Smithe, *"Full-wave Electromagnetic Field Simulation of Lower Hybrid Waves in Tokamaks,"* Radio Frequency Power in Plasmas, Proc. 16th Topical Conf., Park City, Utah, 2005.

K. Wu, J. Ekow, E. J. Otoo, and A. Shoshani, *"An efficient compression scheme for bitmap indices,"* ACM Transactions on

Database Systems, to appear.

K. Wu, J. Gu, J. Lauret, A. M. Poskanzer, A. Shoshani, A. Sim, and W. M. Zhang, *"Grid collector: Facilitating efficient selective access from data grids,"* Proc. of International Supercomputer Conference, Heidelberg, Germany, June 2005.

B. Wylie, B. Mohr, F. Wolf, *"Holistic hardware counter performance analysis of parallel programs short version:,"* Proceedings of Parallel Computing 2005 (ParCo 2005), Malaga, Spain, Sept. 2005.

A. Yamaguchi, *"Chiral condensate and spectral flows on 2+1 flavours Domain Wall QCD from QCDOC,"* Proc. of XXIII International Symposium on Lattice Field Theory (Lattice 2005), 135, 2005.

T. Yamaguchi, *"Entraining cloud-topped boundary layers,"* M.S. Thesis, Colorado State University, 2005.

C. Yang, *"Solving Large-scale Eigenvalue Problems in SciDAC Applications,"* SciDAC 2005 meeting, Journal of Physics: Conference Series, 16, p. 425-434, San Francisco, Calif., June 2005.

C. Yang, W. Gao, Z. Bai, X. Li, L.-Q. Lee, P. Husbands, and E. Ng, *"An Algebraic Sub-Structuring for Large-Scale Eigenvalue Calculation,"* SIAM Journal on Scientific Computing, **27**, 873, 2005.

U. M. Yang, *"Parallel Algebraic Multigrid Methods - High Performance Preconditioners,"* chapter in Numerical Solution of Partial Differential Equations on Parallel Computers, A. M. Bruaset, P. Bjørstad, and A. Tveito, eds., Springer-Verlag, 2006.

L. Yin, X. Luo, M. S. Shephard, *"Identifying and meshing thin section of 3-d curved domains,"* Proc. 14th International Meshing Roundtable, p. 33-54, Springer, 2005.

H. Yu and K.-L. Ma, *"A Study of I/O Techniques for Parallel Visualization,"* Journal of Parallel Computing, **31**, 2, p. 167-183, Feb. 2005.

P. A. Young, C. Meakin, D. Arnett, and C. L. Fryer, *"The Impact of Hydrodynamic Mixing on Supernova Progenitors,"* Astrophysical Journal Letters, **629**:L101-L104, Aug. 2005.

Y. Zhang, X. S. Li, and O. Marques, *"Towards an Automatic and Application-Based Eigensolver Selection,"* LACSI Symposium 2005, Santa Fe, NM, 87501, Oct. 2005.

Y. Zhou, R. Shepard and M. Minkoff, *"Computing Eigenvalue Bounds for Iterative Subspace Methods,"* Computer Physics Comm. **167**, 90-102, 2005.

M. Zingale, S. E. Woosley, C. A. Rendleman, M. S. Day, and J. B. Bell, *"Three-dimensional Numerical Simulations of Rayleigh-Taylor Unstable Flames in Type Ia Supernovae,"* Astrophysical Journal, **632**, 1021-1034, Oct. 2005.

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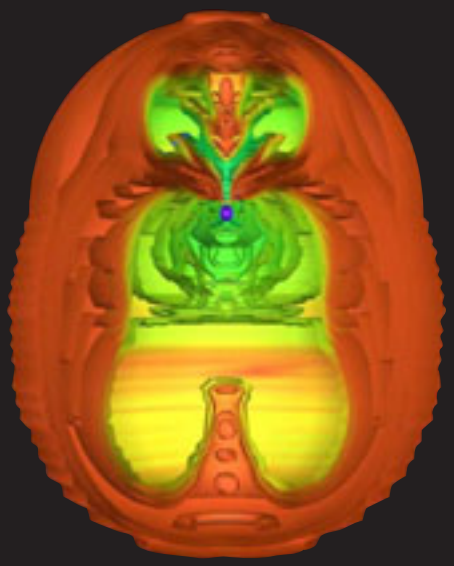

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