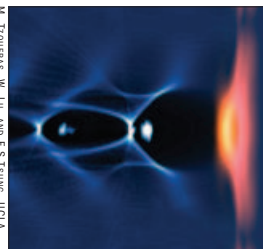


SCIENCE Accomplishments: Results from

Editor's Preface

We present in this article some of the science accomplishments that would not have been possible without the resources of advanced computing, the SciDAC program, and the collaborations that embody the spirit of SciDAC.



M. TZOUFRAS, W. LU, AND F. STIENING, UCCLA

SciDAC is an interdisciplinary program within the Office of Science and SciDAC science spans a spectrum of scientific disciplines ranging from the world of the ultra-small, deep within the atomic nucleus, to the majestic grandeur of stellar and cosmic dynamics. In between these scales, SciDAC programs achieve impressive advances in materials science, nanotechnology, chemistry, biology, geology, environmental science, climate modeling, and more. In addition to basic research, SciDAC also contributes to many applied sciences that rely on advanced computing for precision, predictability, and power.

This second issue of *SciDAC Review* appears in 2006, which has been named the Maxwell Year in honor of James Clerk Maxwell. This follows the Einstein Year (2005), which celebrated Albert Einstein's contributions to science. We would like to start this article on Science Accomplishments by paying tribute to some of the science milestones associated with these doyens. In addition to the direct benefits they have brought to science, technology, and society, Maxwell's equations represent an intellectual marvel: the unification of electricity and magnetism, which were formerly perceived as distinct forces. This was a cornerstone of our attempts to unify all the fundamental forces—a dream that Einstein spent his final days trying to realize. Today, finding the physical basis of Einstein's cosmological constant, revisited in modern science as dark energy, is one of the most challenging problems in physics. Maxwell's equations are still used to describe the fundamental science of fusion plasmas, particle accelerators, and many other areas of basic research and applied science. All these disciplines continue to grow and acquire new insights as

experimental and computational tools grow in power and precision. This evolving, reciprocal relationship between science and its enabling technologies reveals new challenges and opens the door to new horizons for future discoveries.

There have been some radical changes in the way we conduct science and recognize scientists since the days of Maxwell and Einstein. Today it is rare to see an outstanding discovery made by a single scientist. Progress is often achieved through collaborations, which may be national or global, interdisciplinary, or even between science and technology. As the world celebrates the unifying concepts of electromagnetic theory, wave-particle duality, and the space-time continuum, *SciDAC Review* celebrates the unification embodied in computational science. This idea was expressed beautifully in *SciDAC Review* (Spring 2006, p62): "The individual investigator approach has evolved into a tripartite partnership between discipline scientists, applied mathematicians, and computer scientists." In the following sections, we discuss some of the exciting science emanating from such tripartite collaborations.

Deep within the atomic nucleus, quarks and gluons interact by the rules of Quantum Chromodynamics (QCD) and provide clues to the fundamental structures and symmetries of nature. Earlier in this issue ("Quantum Chromodynamics," p5), Nobel laureate Dr. Frank Wilczek emphasized the scientific contributions of lattice gauge theories and computational science to QCD research. In the first section we elaborate on some of the predictions that SciDAC-funded QCD research has made, and the experiments which have verified them.

The exploration of novel ideas and extreme environments has always been a driving force for science. The modeling of high-density plasma environments, in particular, has been integral to the fields of particle accelerator design and modern fusion research ("Simulating Star Power on Earth," *SciDAC Review*, Spring 2006, p40). Interesting results for particle accelerators are addressed in the second section of this article, while the third section discusses an area of fusion research

This evolving, reciprocal relationship between science and its enabling technologies reveals new challenges and opens the door to new horizons for future discoveries.

HIGH-END Computing

where high-end computing and SciDAC funding have provided important results.

While fusion research attempts to realize a source of nuclear energy for the future, high-end computing has also enabled scientists to model combustion and improve the efficiency of conventional fuel burning (p42). The fourth section highlights one of the results achieved in this area. The fifth and sixth sections then discuss important advances in our capacity to predict the properties of bulk materials and nanoscale semiconductor crystals from first principles.

Climate research is vital to ensure our continued presence on Earth, and thus the continuation of scientific research in general. In the seventh section we show how the successful incorporation of biochemical processes into comprehensive climate simulation models enables improved global predictions of climate change. Moving beyond the terrestrial domain, astrophysicists use complex simulations to study the death of stars and the creation of elements essential to life. We close this article with the results for the possible origins of rotation in pulsars produced in supernova explosions.

Dr. Raymond Orbach succinctly described science and why we pursue it in the Spring 2006 issue of *SciDAC Review* (Interview, p8): “Science is a quantitative subject but there is an aesthetic quality to discovery which I think is what drives us. The scientific method is beautiful and structured in itself and it has a vigorous intellectual core.”

Science is interconnected between its multiple disciplines and advances through forward strides in the components as well as by the integral evolution of the whole. Scientific advances through high-end computing and SciDAC-sponsored research add to the foundations of science and promise future expansions. Following in the footsteps of Einstein and Maxwell, SciDAC scientists pursue precision and discovery and SciDAC science adds tripartite collaborations to the ethos of discovery science.

Dr. Lali Chatterjee Editor in Chief, *SciDAC Review*;
Senior Science Advisor and North American Editor, IOP

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QCD: Results from Lattice Quantum Chromodynamics

CONTRIBUTOR: DR. ANDREAS KRONFELD

Lattice QCD predictions for D meson decay have been confirmed by experiment.

Quantum chromodynamics (QCD) is the modern theory of the strong force. In this theory, the main objects are quarks and gluons, which are bound by the strong force into protons, neutrons, and other particles called hadrons. In the framework of QCD, the strong nuclear force binding protons and neutrons together into nuclei is actually only a residue of the much stronger forces acting between quarks and gluons. In fact, inside the proton, even the concept of force is not very useful. Within all hadrons we have a swirl of gluons being exchanged back and forth as a manifestation of the strong force. To make matters worse, gluons can split into two, and then rejoin, or they can split into a quark-antiquark pair. Even the simplest hadron is a complex system hosting constantly interacting components.

Despite this complexity, QCD is well established experimentally. This is because at short distances (or high energies), the coupling between the particles is effectively small and particles move around with relative freedom. This is called asymptotic freedom and QCD is amenable to the traditional methods of quantum field theory in this regime. High-energy experiments have tested and confirmed QCD in this realm, which led to the 2004 Nobel Prize in Physics for Drs. David Gross, David Politzer, and Frank Wilczek, the theorists who provided the theory for short-range QCD and asymptotic freedom.

On the other hand, the traditional methods break down when gluons (and all the complexities that they entail) travel over “long” distances (to particle physicists, the nuclear size 10^{-15} m is a long distance). There is a mathematically rigorous way to handle the gluons in such cases, which is to introduce a grid in space-time—the “lattice” of lattice QCD—and use a computer to keep track of the quarks and gluons on this grid. Of course, the computer does not do everything; the person running the computer has to make sure that the results do not depend on how fine or coarse the grid is. Fortunately, the grid spacing is considered a “short” distance, so on this scale we can use the well-tested methods of perturbative (short distance) QCD.

As is the case for all scientific and computational problems, results need to be tested and validated and we need to be sure that the techniques employed are correct. Physicists from three lattice

QCD collaborations (Fermilab Lattice, MILC, and HPQCD collaborations) decided to address these concerns by making some specific predictions. We used the same methods and input parameters that were used previously with successful results, and set out to calculate the properties of some processes whose measurements were just around the corner.

Our first prediction was for a process very similar to that shown in figure 1. Instead of a B meson the initial state is a D meson, and the final hadron is now a kaon (K). In this case the underlying quark decay is charm to strange ($c \rightarrow s$), which is better understood than $b \rightarrow u$. If we denote the total momentum of the final state electron (e) and neutrino (ν) in $D \rightarrow Ke\nu$ as q , then we predicted that the $c \rightarrow s$ decay rate should depend on q^2 . The q^2 dependence had not been measured when our paper was submitted. Two months later, an experiment called FOCUS published the first measurement of the q^2 dependence of this decay and confirmed our calculation. Since then, the Belle collaboration has completed an even more precise experimental measurement. A comparison between measurement and prediction for the QCD part of the decay (also called the form factor) is shown in figure 2. Our calculation is shown as a curve with an error band, and it is clear that the data points from the Belle experiment fall right on top of this curve.

Another prediction that we made was for a simpler decay of the D meson into just a positron and a neutrino with no daughter hadron. Here a single number, called the decay constant, summarizes the influence of QCD on this process. There are actually two mesons of interest, the D^+ and the D_s ; the latter has a strange (s) quark in it. We finished our work on this decay in June 2005 and the CLEO experiment confirmed our calculation at a conference that July. Since then, another experiment named BaBar has released the first precise measurement of the D_s decay constant. This also agrees with our prediction. A nice way to summarize these results is to take the ratio of the two decay constants, because then several uncertainties from the lattice QCD approach cancel. We predicted that the ratio should be 0.786 ± 0.042 , using lattice QCD, and the experiments described above have found a ratio of 0.779 ± 0.093 .

Long Range Gluons of QCD

There are many problems in particle physics, nuclear physics, and astrophysics that require a quantitative understanding of the connection between quarks and gluons. One of the most basic problems in particle physics, for example, is the experimental quest to understand the interactions between each kind of quark. There are known to be six different types: down, up, strange, charm, bottom, and top. Most of the world is made of up and down quarks, which are confined inside protons and neutrons. But to particle physicists the others are more interesting, because their interactions are intimately related to the origin and evolution of the universe.

The situation described so far is depicted in figure 1. We would like to understand the decay of a bottom (or b, for short) quark, for example, but the b quarks are usually found inside another particle called the B meson. In this environment the b quark will decay to an up (u) quark, and emit (through a virtual W boson) an electron and an antineutrino. No existing experimental apparatus can detect a free quark; instead, we detect the hadron (such as a pion, π) which contains the quark resulting from the decay.

The principal challenge of QCD is to work out the strong, nonlinear interactions of long-range gluons. The best approach, which is already over 25 years old, is to use the lattice formulation of QCD and calculate the

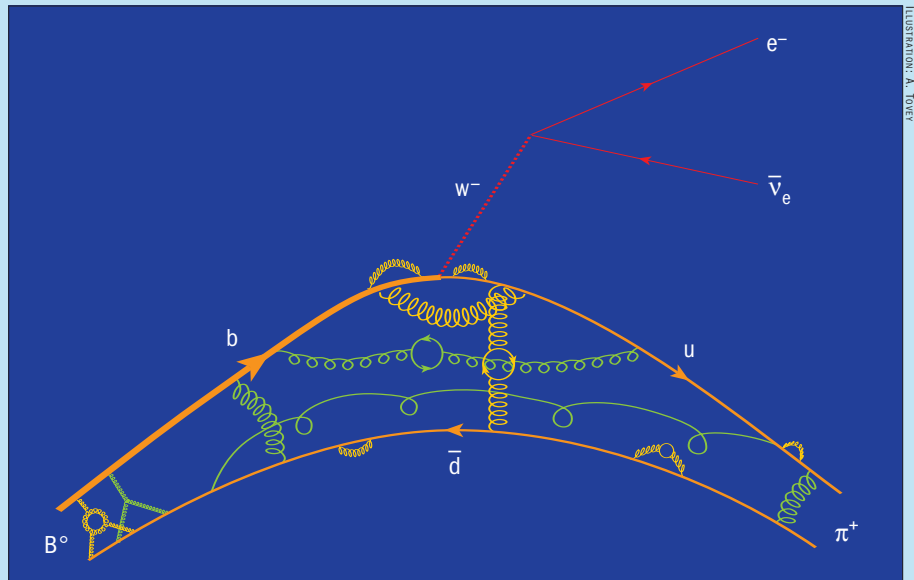


Figure 1. The decay of a neutral B meson. The weak interaction sector (particles connected to the W boson) and the short-range gluons (short coiled lines) can be handled with traditional methods of quantum field theory. The long-range gluons (long coiled lines) need a numerical technique, known as lattice QCD. Recent advances in lattice QCD now include a realistic treatment of the sub-processes in which a gluon turns into a quark loop and back into gluons again.

interactions on a computer. For many years, computing resources were not good enough to simulate one important aspect of these interactions: the tendency of gluons to turn into quark-antiquark pairs, then back into gluons. The situation finally changed at the beginning of

this decade, when a combination of insightful ideas and gains in computing power permitted precise calculations of hadron properties. The predictions that resulted from this work agree with experimental measurements to an accuracy of about 1% or 2%.

The last prediction that we would like to discuss is the mass of an exotic particle called the charmed beauty meson, or B_c . The calculation of its mass tests two aspects of QCD: on one level, our methods for treating the interaction between charmed and bottom quarks; and on another level, our methods for treating the conversion of gluons into light quark pairs. Our calculation obtained a mass of $6,304 \pm 20 \text{ MeV}/c^2$, and was completed before any experiment succeeded in the measurement. In this case, the CDF experiment found a mass of $6,287 \pm 5 \text{ MeV}/c^2$. Figure 3 shows an interesting comparison with previous results. The point on the left is an older calculation that did not include the conversion of gluons into quark pairs and back again. While its range includes the experimental result, it is not constrained enough. It demonstrates that the heavy quarks (charmed and bottom) were being included correctly, but that some other sections may be missing. The modern calculation (middle point) corrects this discrepancy, and is in good agreement with the measurement

from the CDF experiment (right-hand point).

Taken together, these results represent a stringent test of lattice QCD. As in any numerical simulation, there are several ingredients going into our computer code, and each of the three predictions probes a different aspect of the contributing physics. Furthermore, the D decay properties—the leptonic decay constant and the semileptonic form factors—can now be easily adapted to calculate the analogous properties of B mesons, simply by changing the mass of the heavy quark when we run the simulation.

The B meson is one of hottest topics in all of elementary particle physics, and is being subjected to intense scrutiny by experiments at several particle accelerator laboratories. The reason for this intensive study is that the underlying interactions of the b quark are thought to provide important clues about the nature of the universe. How do quarks attain their mass? Or, an even more intriguing question: which elementary processes are responsible for the abundance of matter (and dearth of

Realistic calculation of the charmed B meson mass tests aspects of QCD.

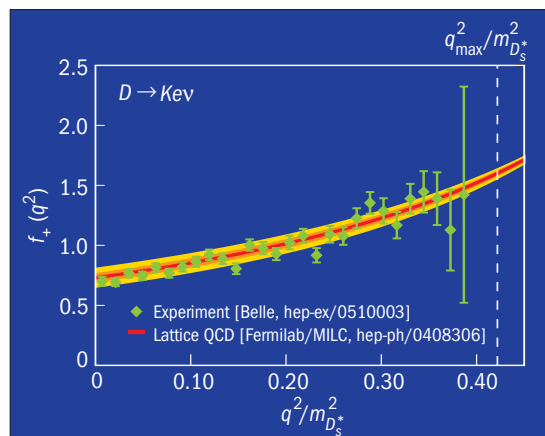


Figure 2. Comparison of the q^2 dependence of the form factor in the decay $D \rightarrow K e \nu$. The error band shows a calculation using lattice QCD and the points give an experimental measurement from the Belle Collaboration.

antimatter) in the universe? The properties of the different quark flavors are connected to yet another mind-boggling question: why is the up quark’s mass a little bit smaller than the down quark’s mass? If it were the other way around (which would fit the pattern seen in more exotic quarks), then protons would decay to neutrons instead of vice versa. A universe with this property would be made only of neutrons, neutrinos, and photons; there would be no atoms, no chemistry, and no life.

The answers to some of these questions may be close at hand. If any of the relevant effects of QCD on B meson decays are large enough, then terascale lattice QCD with an accuracy of 1% or 2% could begin to disentangle the underlying interactions. The harder questions in quark flavor physics—which are related to other overarching questions in particle physics, nuclear physics, and astrophysics—will require even more ambitious numerical calculations at the petascale. Our col-

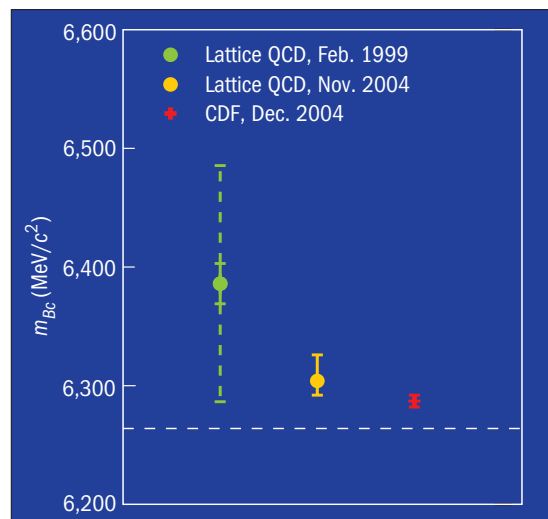


Figure 3. Comparison of the B_c meson mass. From left to right: an old lattice calculation omitting the conversion of gluons into quarks and back; a modern calculation this feature of QCD; an experimental measurement from the CDF Collaboration.

laboration is well positioned to proceed to the challenges and promises of petascale computing. Quantum chromodynamics is one of the most powerful theories of the physical world and the combination of innovative minds and advanced computing resources can utilize its full potential to unravel more of the secrets of science at ultra-small and ultra-large scales.

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PI: Dr. Robert Sugar, University of California–Santa Barbara; work done under the Lattice QCD SciDAC Project

Accelerators: Novel Accelerators Using High-Energy Density Plasmas

CONTRIBUTOR: DR. WARREN MORI

The long-term future of experimental high-energy physics research using accelerators can be strengthened by the successful development of novel ultra-high-gradient acceleration methods. New acceleration techniques using lasers and plasmas have already exhibited gradients and focusing forces more than a thousand times greater than conventional technologies. The challenge is first to control these high-gradient systems, and then to string them together. This technology

could enable the development of ultra-compact accelerators, which could be used in industry and medicine as well as science. The potential impact of this advancement is truly staggering. In addition, plasma-based acceleration is just one aspect of a rapidly emerging field called high-energy density plasma physics. The on-focus energy density of the particle beam drivers and laser drivers used in this field approaches 1 Tbar of pressure. When such beams interact with plasma or un-ionized

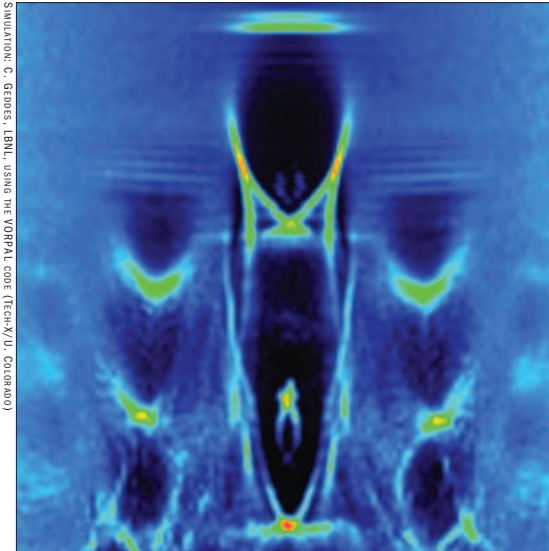


Figure 4. Shown above is plasma density, including the wake and trapped particle bunches (bright dots on black, on the center line), in a channel-guided wakefield accelerator from a SciDAC simulation using the VORPAL code. Particles are trapped, followed by loading of the wake by the trapped bunch, and concentration of the particles in energy when the higher energy particles outrun the accelerating structure.

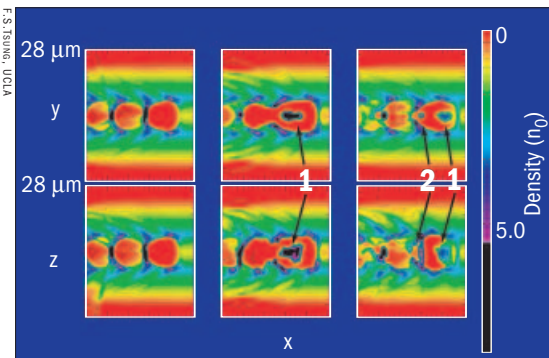


Figure 5. A sequence of 2D cuts through the 3D data of the electron density. The laser is propagating from left to right. After 0.24 cm (left column) there are no self-injected electrons. After 0.43 cm (middle column) the self-injected electrons are seen. The electron beam shape is different in the two planes (xz and yz), an effect which has been seen experimentally. After 0.64 cm the first bunch has completely outrun the plasma wave and a second bunch has been injected.

matter, the physics involved includes ultra-fast, relativistic, and nonlinear phenomena.

Three independent experimental groups have recently observed the creation of ~ 100 MeV monoenergetic beams carrying ~ 100 pC of charge, when a ~ 10 TW laser propagates through ~ 1 mm of plasma at densities of $\sim 10^{19}$ cm $^{-3}$. We would like to understand the nonlinear evolution of the laser, capture the self-injection of the electrons, and study how the electrons can be accelerated to form monoenergetic beams. For such a complex problem, sim-

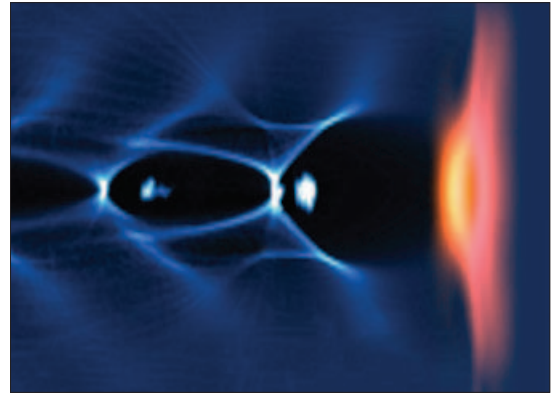


Figure 6. A 2D slice of a 3D simulation showing the laser envelope (in orange) and the plasma density (in blue). As the laser moves from right to left it blows out the electrons, which rush back to the axis once the laser has passed. There they feel a strong accelerating force and are self-injected in the laser's wakefield. They are accelerated until they outrun the wake.

ulations that follow the trajectories of individual particles (particle-in-cell methods) are required. Each of the published results mentioned also discusses supporting simulations; indeed, unraveling the underlying physics is not possible without fully nonlinear simulations of the particles involved. Two massively parallel particle-in-cell codes, OSIRIS and VORPAL, have been used to elucidate the key physics in these experiments. A sample result from a VORPAL simulation is shown in figure 4.

In addition, prior to these experiments, 3D OSIRIS simulations had already predicted that a modest 13 TW laser could indeed self-inject electrons. As the laser evolves, a combination of frequency redshift and group velocity dispersion can produce a monoenergetic beam; the electrons in the forefront of the beam dephase into a decelerating region, while those in the back continue to be accelerated by the beam. The parameters of these simulations were not identical to those of the cited experiments, but they succeeded in predicting the essential physics. This physics is illustrated in figure 5, which shows the evolving plasma density in 2D slices through the 3D data. Within the next three years, laser power will increase from ~ 10 TW to 1 PW. Full-scale 3D OSIRIS simulations at these energies have already been carried out, and predict that a 200 TW laser should produce a 1.5 GeV monoenergetic beam with 0.5 nC of charge. This simulation followed 0.5×10^9 particles on a $4000 \times 256 \times 256$ grid over 300,000 time steps. Figure 6 shows a 2D slice through the laser and plasma density from this simulation.

Contributor: Dr. Warren Mori, on behalf of SciDAC's Advanced Accelerator Group; work done under SciDAC AST project

Fusion: Using Electromagnetic Wave Conversion to Control Fusion Plasmas

CONTRIBUTOR: DR. PAUL T. BONOLI

One of the interesting properties of magnetized plasmas is that at any given frequency, several different kinds of plasma waves with very different wavelengths can coexist. If the wave frequency is near the ion cyclotron frequency, then a fast, long-wavelength wave launched into a non-uniform plasma can, over a short distance, couple to a short wavelength ion Bernstein wave (IBW) and an ion cyclotron wave (ICW) through a process known as mode conversion. The fast wave and the ion cyclotron wave are similar to light waves, in that their polarization is nearly perpendicular to their direction of propagation. The ion Bernstein wave is similar to a sound wave, in that its polarization is nearly parallel to its direction of propagation. Now, with the help of terascale computers and algorithms developed in our SciDAC project, we are able to solve the wave equations for plasmas with 2D spatial variations at sufficiently high resolution to study mode conversion. Figure 7 shows one component of the AORSA2D code's solution for a wave's electric field, following the propagation of fast waves launched from an antenna on the right (not shown) into the Alcator C-Mod tokamak at MIT. The large-scale structure in the left-hand panel is the fast wave. The curved blue line (seen more clearly in the magnified view to the right) is the mode conversion layer. The figure shows a conversion to one kind of short-wavelength mode, an IBW, propagating to the left near the horizontal mid-line. There is also some conversion to a completely different type of short-wavelength mode (slow ICW), however, which can be seen above and below the mid-line propagating to the right. It had previously been expected that the dominant conversion would be to an IBW wave, which would propagate only to the left of the conversion surface.

This process has been observed experimentally on the Alcator C-Mod tokamak, using an innovative new diagnostic technique called Phase Contrast Imaging (PCI). PCI measures the density fluctuations associated with mode-converted waves. The PCI measurements are integrated along a vertical chord through the plasma. These

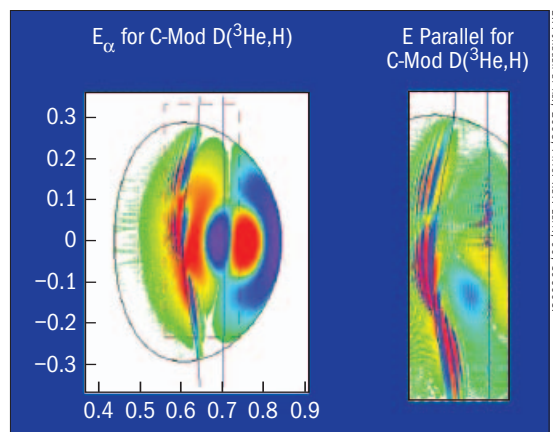


Figure 7. Wave electric field for mode conversion in the Alcator C-Mod tokamak, computed with the AORSA2D code.

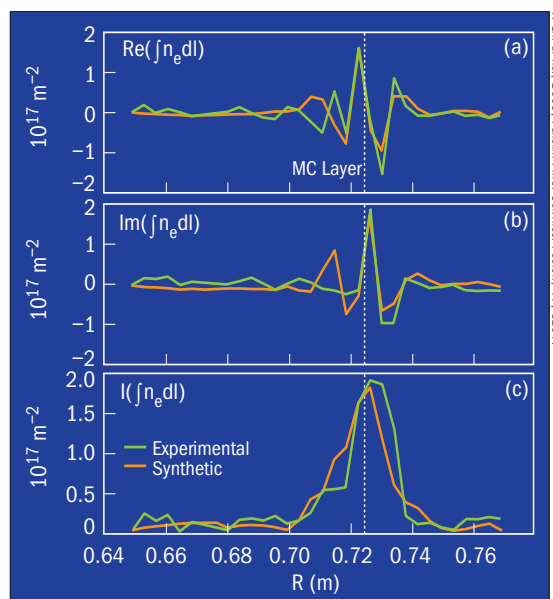


Figure 8. Comparison of the line-integrated density from the PCI diagnostic and a synthetic diagnostic prediction using wave electric fields from the TORIC code.

Alcator C-Mod measurements have been modeled extensively using the TORIC code, incorporating a “synthetic diagnostic” to predict the signals observed by PCI instruments. Figure 8 shows the in-phase and quadrature components of this prediction, as well as a comparison between the modulus of the line-integrated experimental density

perturbation and the TORIC prediction. The results are in good agreement with respect to the spatial structure and spectrum of the wave.

The fusion program is actively developing techniques to make use of these mode-converted waves, which may be able to control the current and pressure profiles in fusion devices. Ion Bernstein waves are absorbed primarily by electrons, and are effective in driving the current. The slower ion cyclotron waves, on the other hand, are absorbed mainly by ions and should be more effective in driving plasma flow and improving confinement. Given these potential uses, our results are extremely encouraging; they increase our confidence in the capacity of our models to accurately simulate mode conversion in a tokamak. More generally, these simulations demon-

strate the feasibility of solving a problem containing processes at disparate spatial scales. The techniques used by our simulations could be applied to other areas of physics, such as wave propagation in the Earth's magnetosphere.

If petascale computing resources were available to this project, it would also be possible to assess the feasibility of using mode-converted ICRF waves for plasma control in the planned ITER device. We would also be able to simulate 3D plasma confinement devices such as stellarators.

Contributor: Dr. Paul T. Bonoli, MIT Plasma Science and Fusion Center, on behalf of the SciDAC Center for Simulation of Wave-Plasma Interactions (CSWPI)

PI: Dr. Paul T. Bonoli

Combustion: Near-Wall Heat Transfer in Gas Turbine Combustors

CONTRIBUTOR: DR. JACQUELINE CHEN

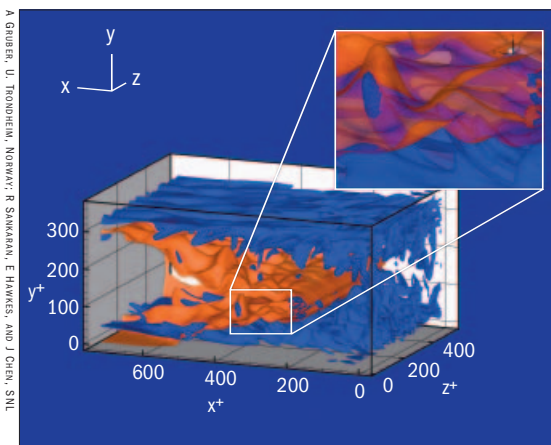


Figure 9. Instantaneous snapshot from DNS of a hydrogen-air, V-shaped, premixed flame immersed in a turbulent Poiseuille flow as it interacts with the channel walls. Flow is from right to left. A temperature isocontour representing the flame is shown in red and a vorticity magnitude isosurface is shown in blue.

It is critical to understand the process of near-wall heat transfer in designing gas turbine combustors. It is likewise important to accurately estimate the spatial and temporal patterns of heat flux to the wall, which are related to combustion processes in the turbulent boundary layer, because the thermal stresses induced by transient heat transfer into the wall material can affect the combustor lifetime. Sandia combustion researchers supported

by SciDAC and other Office of Science programs, along with collaborators from the University of Trondheim in Norway, have performed three-dimensional Direct Numerical Simulations (3D DNS) to study the evolution of an anchored, hydrogen-air, V-shaped, premixed flame, immersed in a turbulent Poiseuille flow, as it interacts with the channel walls. The simulations were performed with detailed hydrogen-air chemical kinetics, and allowed to run as long as was necessary to reach statistical stationarity. The 3D DNS results reveal that the formation of near-wall coherent turbulence structures shaped like hairpins, which push the flame towards the wall on one side and away from it on the other (figure 9), thereby inducing large spanwise gradients of heat flux to the wall. By examining temporal and spatial scalar spectra, the researchers discovered that the characteristic spatial and temporal pattern of wall “hot spots” is correlated with the passage of these hairpin-shaped vortical structures. Moreover, they discovered that, as the flame quenches near the wall, an exothermic radical recombination reaction which produces hydroperoxy also contributes significantly to the heat flux to the wall.

Contributor: Dr. Jacqueline Chen, Sandia National Laboratories (SNL), on behalf of Dr. Andrea Gruber, SNL and University of Trondheim, Norway

Materials Science: Quantum Simulations for Molecular and Material Properties

CONTRIBUTOR: DR. GIULIA GALLI

In the field of materials science and chemistry, one of the Grand Challenge problems for the next decade is the prediction and design of molecular and material properties with controllable accuracy, from first principles; that is, from the fundamental laws of quantum mechanics. This can be accomplished by using advanced quantum simulations (QS), which provide numerical solutions to the partial differential equations representing the laws of quantum mechanics. In QS, the interaction between electrons and ions is modeled in an approximate, non-empirical manner. The last thirty years has seen key progress in the fundamental theories of condensed matter and molecular systems, the development of algorithms implementing both mean field and stochastic approaches, and the creation of optimized simulation codes running on high-performance computers. All these advances have transformed QS into a powerful tool capable of addressing the complexity of materials and nanostructures at the microscopic level. Numerous material properties can now be inferred from the fundamental laws of quantum mechanics without any input from experiment, and in some cases one can even investigate conditions not yet accessible.

Over the next decade we expect QS to acquire a central role in materials science and chemistry, as further theoretical and algorithmic developments allow the simulation of a wide variety of condensed and molecular systems with specific, targeted properties. This will open up the possibility of predicting and designing optimized materials and nanoscale devices from first principles. Although this modeling revolution will be years in the making, its unprecedented benefits are already becoming clear. Indeed, QS applications are currently making key contributions to our understanding of nanoscale measurements, complex, disordered systems (including liquids and solids under extreme conditions), and composite organic/inorganic materials. A fundamental understanding of microscopic behavior is very much needed in the field of nanoscience, where experimental investigations are often controversial and cannot be explained on the basis of sim-

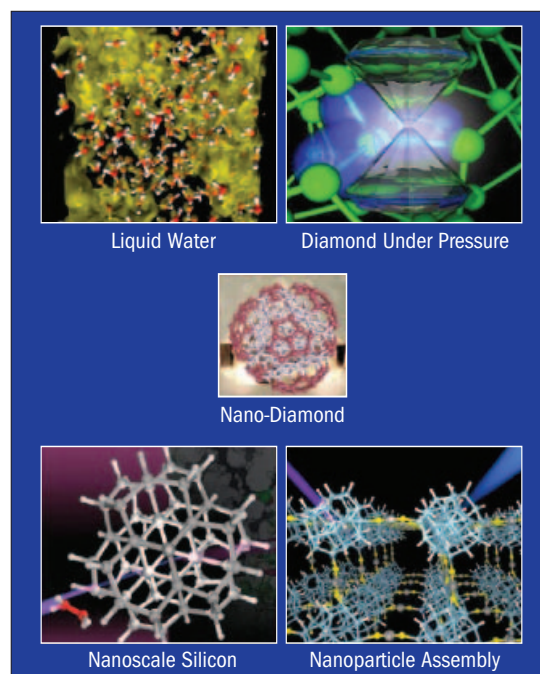


Figure 10. This figure shows “ball and stick” representation of nanostructures (bottom panels) and fluids (upper panels) investigated using quantum simulations. In particular, a model of a silicon dot (left) and of an array of Si nanoparticles are shown in the lower part of the figure, and both atomic positions and electronic states are presented in the upper part for liquid water (left) and compressed diamond (right).

ple models. It is just as important in the study of materials under extreme conditions, for which experimental data are usually rather limited. Some examples of recent predictions obtained using QS are illustrated in figure 10, where we use the “ball and stick” representation of microscopic structure for solids (diamond under 1,000 GPa of pressure), liquids (liquid water), and recently synthesized nanostructures (silicon and carbon). For all these materials, QS applications have provided a deeper understanding of their structural, optical, and vibrational properties, and have guided the interpretation of key experimental data.

Contributor: Dr. Giulia Galli, University of California–Davis

Applied Energy Sciences: Connecting the (Quantum) Dots

Predicting the Electronic Structure in Networks of Nanodots and Wires

CONTRIBUTOR: DR. ALEX ZUNGER

Over the past decade, research efforts have produced revolutionary breakthroughs in both the synthesis and characterization of quantum dots. Quantum dots are small nanoscale (order of 10^9 meters) particles that contain between a few thousand and one million atoms. We now know that changing the size of materials—going down to nanosize—can dramatically alter intrinsic material properties, such as converting a conductor into an insulator or a nonmagnetic material into a magnet.

Research Fellow Dr. Alex Zunger heads a team of researchers from the National Renewable Energy Laboratory (NREL), Lawrence Berkeley National Laboratory (LBNL), and University of Tennessee. Funded by the Office of Science, the group has been focusing on the physics and computational challenges of simulating the electronic properties of quantum dots and quantum dot architectures. Due to the very large number of atoms involved, conventional numerical applications of quantum mechanics are impractical. The SciDAC team has developed new and improved algorithms, as well as better preconditioners, to overcome this obstacle.

A quantum dot confines the electrons to discrete energy levels that can be controlled by changing the size and shape of the quantum dot. These properties make quantum dots potentially important in a number of areas, such as diode lasers, advanced quantum computing, and ultra-high efficiency solar cells. However, the promise of such dots depends largely on the ability to connect, or wire together, different dots. This raises fundamental quantum-mechanical questions. Will the electrons in a dot connected to another dot by a nanowire be confined to a single dot (become localized)? Or will the electrons be predisposed to move along the wire (become delocalized)?

What makes the problem involving motion of electrons from a dot to a wire and then to another dot difficult is the quantum behavior. For example, if the dot is sufficiently small, electrons in it will be squeezed for space—quantum confinement—and seek to move away into the wire. However, the existence of another electron in the

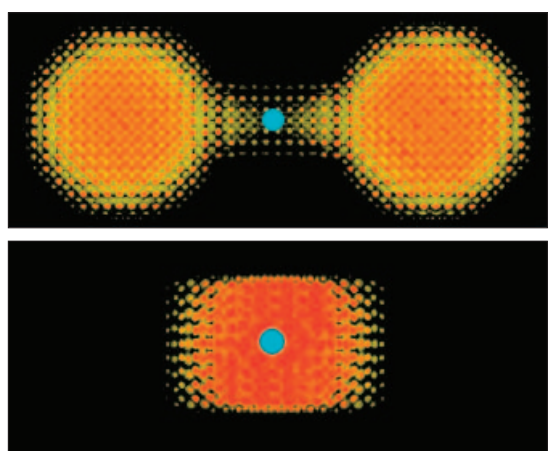


Figure 11. If one connects two cadmium telluride (CdTe) dots by a 20 Å diameter cadmium selenide (CdSe) wire and then places one electron on the wire (upper panel), the second electron (shown as yellow clouds) will be spread on the two dots. On the other hand, if the wire connecting the dots is just a bit larger, 30 Å in diameter (lower panel), then placing one electron on the wire attracts the second electron to the wire.

wire will repel the electron back into the dot—quantum correlation. To find out who wins, quantum confinement or quantum correlation, powerful new computational techniques are needed. The Zunger-led team has developed such methods to handle both quantum confinement and quantum correlation, and they have applied the methods to a “nano-dumbbell” consisting of two dots connected by a wire. They found that, while electrons could get stuck in the dot, one could design certain dimensions of wires and dots that would facilitate electron delocalization. Figure 11 demonstrates this for cadmium telluride (CdTe) dots. A ten angstrom (Å) difference in size can delocalize electrons from individual dots. Such breakthrough calculations enable the design of three-dimensional quantum architectures—wired-up dots that can exploit the wonderful properties of the nanoworld.

Contributor: Dr. Alex Zunger, Research Fellow, National Renewable Energy Laboratory; PI on the project, “Predicting the Electronic Properties of 3D, Million-Atom Semiconductor Nanostructure Architectures”

Climate: Predictions from Improved Models

CONTRIBUTOR: DR. PHILIP JONES

The SciDAC project, “Collaborative Design and Development of the Community Climate System Model (CCSM) for Terascale Computers,” was launched to accelerate the development of the CCSM.

The Community Climate System Model (CCSM) is a coupled climate model, consisting of four components for the Earth’s atmosphere, ocean, sea ice, and land surface. Each model component communicates its surface fields and fluxes to the other components through a flux coupler. The CCSM is used for climate change research and to provide periodic Intergovernmental Panel on Climate Change (IPCC) climate assessment reports.

The SciDAC project, “Collaborative Design and Development of the Community Climate System Model (CCSM) for Terascale Computers,” was launched to accelerate the development of the CCSM. Over the past five years, six DOE laboratories and researchers from the National Center for Atmospheric Research (NCAR) and the National Oceanic and Atmospheric Administration (NOAA) have worked together on a variety of improvements to the CCSM. These improvements include advancements in software design and engineering, the introduction of new numerical algorithms, and the addition of new physical processes to the CCSM models.

The early stages of this project focused on improving the performance of the CCSM and its portability to a wide variety of vector and scalar computer systems. Flexible data decomposition schemes in the atmosphere and ocean models were introduced to enable the necessary fine-tuning for each platform. The sea ice and land model components were also restructured to improve their performance, particularly on vector computers. Finally, new software was developed to improve the coupling of all four components and produce a fully coupled model. Thanks to these improvements, CCSM scientists were able to produce the world’s largest ensemble of climate simulations for the recent IPCC assessment. This ensemble contains over 10,000 years of data simulated at relatively high resolution.

The SciDAC CCSM consortium has also contributed new model algorithms and new scientific capabilities to the community. The consortium participated in the creation of a new finite-volume method for simulating atmospheric dynamics, and also developed a new numerical formulation useful for ocean models.

Until recently, the concentrations of greenhouse gases and atmospheric aerosols have been specified as parameters of the model, whose values are based

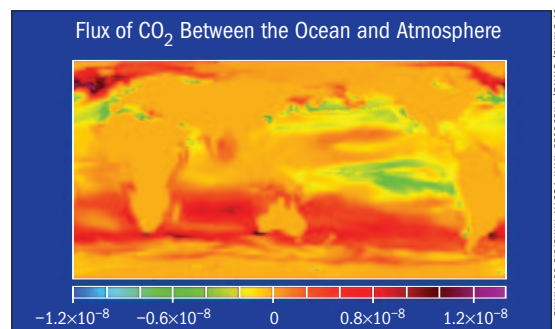


Figure 12. Sources (red) and sinks (green) of atmospheric CO₂ from ocean ecosystems as simulated by a prototype biogeochemistry version of the Community Climate System Model (CCSM). Coupling the carbon cycle with models of global climate dynamics will help determine the safe levels of atmospheric greenhouse gases.

on the future rate of fossil fuel consumption, the ability of oceans and land to adjust to change, and other assumptions. In recent years the project has primarily focused on adding the carbon and sulfur cycles to the climate system model. By introducing the biological and chemical processes that govern the absorption and emission of greenhouse gases, we can better simulate the response of Earth’s climate system to human emissions. A prototype carbon-climate-biogeochemistry model has now been assembled, as a practical demonstration of coupled Earth system simulations at this dramatic new level of complexity. This new model includes a comprehensive formulation of atmospheric chemistry, as well as land and ocean ecosystem models. In this first step towards a truly comprehensive Earth system model, each component exchanges CO₂ fluxes with the others. In addition, the ocean component supplies a flux of dimethyl sulfide (DMS), which is used by the atmospheric model to create sulfate aerosols. These aerosols interact with and influence the physical climate system, the oceanic carbon cycle, and terrestrial ecosystems. This prototype model, which was developed under SciDAC, will form a basis for future work towards a comprehensive Earth system model and enable climate researchers to more realistically simulate future climate change and its impact.

Contributor: Dr. Philip Jones, Los Alamos National Laboratories (LANL)

PIs: Dr. John Drake, ORNL; Dr. Philip Jones, LANL

Astrophysics: Generation of a Neutron Star Spin Period of 50 ms in a 3D Supernova Simulation

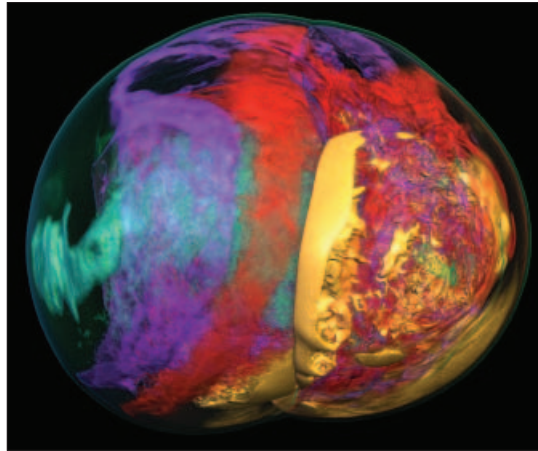
CONTRIBUTOR: DR. JOHN BLONDIN

The origin of pulsar (rotating neutron star) spin is still unknown. Neutron stars, and therefore pulsars, are born in core collapse supernovae explosions. Given their role as one of the most important sources of elements in the universe, understanding how such explosions occur is one of the most important unsolved problems in astrophysics. The generation of spin in our 3D modeling of core collapse supernova explosions points to a new mechanism for the origins of pulsar spins. The supernova shock wave is unstable and in 3D, this instability leads to a rotating flow below the shock. This results in the deposition of angular momentum onto the forming neutron star. The spin period we obtain is within the range of observed pulsar spin periods. Previous explanations relied solely on the evolution of the stellar core's initial rotation as the core collapses during the supernova. Consequently, there was an artificial one-to-one mapping between initial stellar rotation and final neutron star spin, artificially constraining the former.

Precision observations of neutron star radii and masses allow neutron stars to serve as laboratories for fundamental nuclear physics not accessible to terrestrial experiments. Observations of pulsar orbital decay by the emission of gravitational waves have provided indirect evidence of such waves, predicted by Einstein's general theory of relativity, further motivating direct searches by LIGO and other gravitational wave observatories for gravitational waves from core collapse supernovae and other sources.

Our 3D results also demonstrate how different the outcomes in 3D and 2D simulations of core collapse supernovae are, demonstrating in turn that full 3D models are required to ascertain the core collapse supernova explosion mechanism and to predict all of the observables associated with such supernovae and their remnants. Our results on neutron star spin could not have been obtained in 2D models, where the imposition of artificial symmetries (axial symmetry) reduces the number of degrees of freedom and thereby restricts the possible simulation outcomes. Nature imposes no such symmetries.

Our 3D results further demonstrate the efficacy



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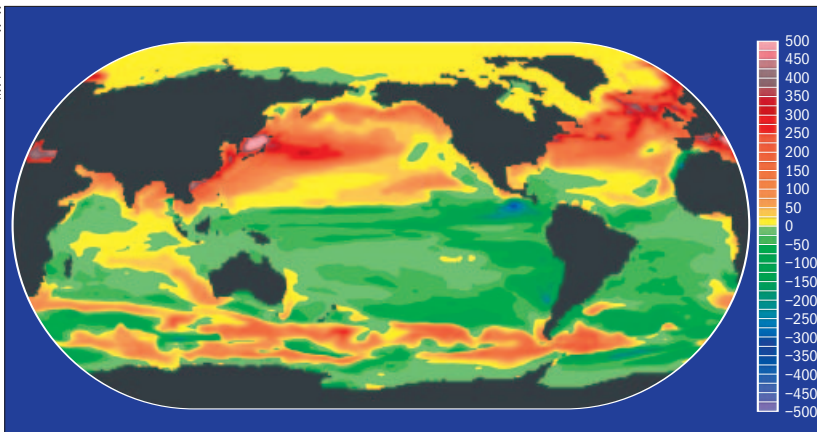
Figure 13. The angular momentum in the 3D stellar core flow below the supernova shock wave is depicted in this image. The outer surface is the shock wave. Evident are two large counter-rotating flows, one just below the shock, shown in gold, and the other in the deeper region above the forming neutron star, shown in green. The angular momentum in the inner region is deposited on the neutron star, spinning it up. This mechanism may be responsible for the birth of pulsars (rotating neutron stars). The simulation shown here was performed by Dr. John Blondin (NCSU) on the ORNL Leadership Computing Facility.

of scientific computation at the terascale and, ultimately, petascale for scientific discovery. It can be argued easily that discovery in the context of non-linear, multiphysics applications such as ours and the solution of some of nature's Grand Challenge problems will not be achieved in any other way.

With petascale platforms, our 3D hydrodynamics-only simulations can be advanced significantly, allowing full 3D multiphysics simulations of core collapse supernovae. At this scale, the explosion mechanism for core collapse supernovae will finally be ascertained, as well as the underlying mechanism for neutron star spin and other observables associated with core collapse supernovae and the neutron stars they produce.

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PI: Dr. Anthony Mezzacappa, ORNL



A further example of climate research (p22). The image shows CO_2 gas flux (in kilotonnes/ km^2 /year) between the ocean and atmosphere averaged over December of year 9 of the fully coupled chemistry simulation. Positive values indicate uptake by the ocean; negative values indicate outgassing into the atmosphere. The ocean uptake in the Southern Ocean is due to a seasonal phytoplankton bloom.

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