Cover: As physicists seek to solve the complicated equations of quantum chromodynamics, they are turning to custom-built supercomputers. The approach corresponds to hard-wiring the interactions of quarks and gluons on circuit boards.

Illustration: Sandbox Studio
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China has about 100 million Internet users today. US particle physicists brought the first Internet connection to China in 1994.

ibc Logbook: Inventing the Web
In March 1989, Tim Berners-Lee wrote a memo with the title “Information Management: A Proposal,” the blueprint of the Web.

bc 60 seconds: The Grid
Like its electrical namesake, a computing grid is a mix of technology, infrastructure, and standards.
My first computer, as a child, was a Commodore VIC-20. I learned to program on it but within weeks had exhausted its 5-kilobyte memory. My initial frustration led to a realization that I needed to use the resources more efficiently, and so I managed to squeeze much more performance out of the machine. Soon, my ambitions exceeded the resources I had on hand. The next generation of home computers came along soon, and the 64-KB memory of the Commodore 64 kept me busy for a little longer. As IBM PC clones became readily available, personal-computer advances seemed to speed up—I was witnessing Moore’s Law at work. The memory and processor speed of a modern home computer are almost exactly what Moore’s Law predicted since I first started computing—a doubling in power every two years.

Just as home computing is advancing rapidly, so is high-end computing, tied closely to advances in science. This issue of *Symmetry* examines computing advances in relation to particle physics, in time for SC05, the premier international conference for high-performance computing.

Particle physicists have always been among those at the leading edge of computer development. They use the latest software and hardware in almost all aspects of their work, from designing experiments to collecting and analyzing data. Physicists have consistently shown that they can use the extra computing resources effectively and efficiently, often pushing the limits of discovery.

To collect data from CERN’s Large Hadron Collider, computing resources need to exceed current availabilities by a vast amount. To handle all the data, physicists and computer scientists are developing new infrastructures and techniques such as grid computing, a method for sharing resources over global networks.

Meanwhile, understanding the floods of data to come from LHC will require improvements in theoretical understanding. Making precise predictions with quantum chromodynamics, the theory of the strong force that mediates quark interactions in LHC collisions, is notoriously difficult. One approach to the problem is a computer-intensive technique called lattice QCD. Physicists designed custom chips to perform the lattice calculations, and those chips have since found further application in IBM’s Blue Gene/L supercomputers, used to study biological processes.

Biologists, climatologists, geologists, and many other scientists are increasingly using high-end computing. But even as more sciences take advantage of computing advances, the symbiosis between physics and computing will continue, driving Moore’s Law until physics has a different kind of influence on computing.

When the structures on computer chips shrink so that quantum effects dominate, a new type of computing will take over. Perhaps the next generation of computer-savvy children will be hacking a new era of quantum computers, learning to drive computation and physics to further advances.

David Harris, *Editor-in-Chief*
Scientific Computing

The future of science will be driven by the improving performance of accelerators, telescopes, microscopes, spectrometers, and computers. The progress of scientists will depend on how well these instruments leverage each other and the investigation process. Huge data sets threaten to overwhelm researchers in physics, chemistry, biology, climatology, and cosmology; bigger data sets are on the way as spatial resolution and sampling frequencies improve. Extracting knowledge from this “data tsunami” is the first priority of scientific computing.

The interactive visualization of massive data sets is perhaps the most useful approach. Auditorium-level visualization allows for multi-disciplinary viewing and interaction between investigators; remote viewing and control can be achieved without having to transmit any of the data set. Interactive immersion within the data itself encourages discovery and exploration of singularities, discontinuities, artifacts, and irregularities that may not be obvious otherwise. New and insightful questions easily arise in this viewing environment because it is very intuitive.

Very large, complex models are readily viewable in this manner: the complete structure of a Boeing 747 aircraft, the seismic data of an underground oil and gas reservoir, and the 60,000 CT scans of a 2000-year-old Egyptian mummy.

Multi-level, multi-physics models can be merged into a common operating picture to enhance decision making, analysis, and discovery. This has been of real value to defense and homeland security analysts, and will soon become a necessary tool for natural disasters’ prediction and response planning.

Nature is complex, non-linear, and non-homogeneous. The modeling, simulation, and visualization of her secrets require immense amounts of compute power, software capability, and data capture. Fortunately, we have Moore’s Law and parallelism on our side. The rate of advance in compute power exceeds anything else in human experience.

More recently, emerging satellite and fiber-optic networks can be used to build computerized scientific instruments that straddle the globe. As for the architecture that binds the myriad of compute elements together, there will always be multiple choices. However, given that scientific data is generally real-time streaming data, it is essential that all data paths have high bandwidth and low latency characteristics.

Having large amounts of memory will help sustain modeling and simulation activities that may be taking place contemporaneously with data collection. NASA’s space shuttle turbine, for example, creates 50 terabytes of data per second during shuttle-launch simulation. And the recently installed Altix supercomputer at Japan’s Atomic Energy Research Institute includes 13 terabytes of globally-shared memory to simulate nuclear fusion.

Modeling, simulation, and visualization together create a third branch of human knowledge, perhaps on equal footing with theory and experiment, and the predictive power of mathematical models is accelerating scientific discovery. Rapidly increasing compute capabilities allow for finer granularity and model refinements: climate models now take into account terrain, rivers, lakes, vegetation, dust, cloud cover, and ocean salinity. The computer industry is striving to meet the challenge of nature’s additional complexities. Japan’s Earth Simulator, built by NEC and first operated in 2002, was considered a “Sputnik” event at the time. It delivered 35 teraflops of sustained performance, but was later superseded twice by more powerful US-built machines (first by SGI at NASA Ames, then by IBM at Lawrence Livermore National Laboratory). More importantly, the Earth Simulator has triggered a race to petascale performance levels, most likely achievable by the end of this decade.

In the next generation of supercomputers, new processing elements will augment the traditional ones, all fully integrated onto large amounts of globally-addressable shared memory, and all under the supervision of a single operating system, most likely Linux. Such machines will “reconfigure” themselves on the fly, and optimize their compute elements for the code at hand. They will form the high-performance nodes of larger grids, both national and international, that make up the compute platform and cyber-infrastructure for science in the next decade.

Beyond that, Moore’s Law will reach its limit as semiconductor line widths approach the dimensions of a single atom, in which case “quantum computing” may kick in to boost performance for many machine generations yet again. By the middle of the 21st century, we will be ready to model the human brain and mimic its extraordinary thinking abilities. Consistently, scientists and engineers will find a way to out-compete in order to out-compete.

Bob Bishop

Bob Bishop is Chairman and CEO of SGI. His 40-year globe-spanning career involves active partnering with scientists and engineers in their efforts to accelerate discovery and innovation.
Tevatron sets world record; the most productive age for research; numbers: Pierre Auger Observatory; bicycle networks; keeping computers cool; opera review: Doctor Atomic.

A bright machine
The Fermilab Tevatron achieved a world-record peak luminosity, or brightness, in colliding protons and antiprotons on October 4, 2005. The luminosity of $1.4\times10^{30} \text{ cm}^2\text{sec}^{-1}$ is about four times the luminosity achieved three years ago, and more is expected to come.

To maximize the potential for scientific discovery, accelerator experts improve and tune their machines to produce the largest number of collisions per second, a rate known as the peak luminosity of a particle-collider machine.

The Tevatron record surpasses that set in December 1982 by the ISR collider at CERN, which collided protons on protons. The ISR achieved a peak luminosity of $1.40\times10^{30} \text{ cm}^2\text{sec}^{-1}$ at a collision energy of 62 GeV.

Why did it take 23 years to break the ISR record? Beams of antiprotons are much harder to produce than protons, and the Tevatron operates at a much higher collision energy of 1960 GeV. The Tevatron record is tied to the startup of a new technique to cool antiproton beams, which makes the beams more concentrated. Kurt Riesselmann

Don’t cite anybody over 30?
A common assertion is that the best work in physics is done by people who are under 30. Is it true? This chart shows the ages of authors at the date of publication of the top 25 theoretical papers from the SPIRES all-time top-cited list. Included are the 29 authors whose ages are in the database. Some appear more than once as authors on multiple papers.

Half the authors were 32 or younger when they published their famous papers. The chart shows that the most frequent ages are 29 and 30. In fact, almost half the ages are concentrated around the window of 29-30.

Heath O’Connell, Fermilab

Ages at publication of top-cited papers

Numbers: Pierre Auger Observatory
In November, the Pierre Auger Observatory outside Malargüe, Argentina, celebrates its scientific launch. The observatory will record high-energy cosmic-ray showers with ground-based water tank detectors and air-shower cameras.

David Harris

3000 Detector area in square kilometers

30 Number of times Paris would fit within detector area

1400 Meters above sea level

739 Current number of water tanks

1600 Eventual number of tanks

11,000 Liters of water per tank

1500 Meters between water tanks

20 Years of expected lifetime for tanks

3 Current air observation cameras

440 Photomultiplier tubes per camera

1500 Events per day recorded

140 Highest energy of a recorded event in EeV (exa-electronvolts = 10^{18} eV)

100 Speed in miles/hour of tennis ball with equivalent energy

15 Countries participating

1938 Year Pierre Auger discovered cosmic ray showers

20,000 Population of Malargüe

927 Argentina’s average human population per detector area

81 Argentina’s average llama population per detector area
Networks of the past

In today’s particle physics experiments, it takes a fraction of a second for data recorded by detectors to be transferred to a data storage facility. Soon thereafter, collaboration members from around the world have access to the data via the Internet.

Not so thirty years ago. In the 1970s, experimentalists at Fermilab and other labs had no networks to transfer their experimental data from the data acquisition system to the places where they would store and analyze their data. Their mode of data transfer was rather low-tech: the bicycle. At the end of a shift, a scientist would take the tapes with data, hop on a bike, and ride over to the computer center or wherever the data analysis took place. This process even received its own acronym: BOL, for “Bicycle Online.”

Today, the Bicycle Online transfer is history. But like thirty years ago, Fermilab again has a pool of bicycles that is available for experimenters to ride around the site. But today’s bike trips are usually to meetings and seminars, or just out to lunch.

Kurt Riesselmann

Hot computers

Computing centers are hot—literally. At least, they are in the absence of extensive cooling systems. With an increasing number of computers installed at scientific labs nationwide, the efficiency of those cooling systems is becoming much more important. Just ask John Weisskopf, technical operations manager at the Stanford Linear Accelerator Center. He is responsible for keeping the more than 3500 computers in the laboratory’s main computer center from overheating.

The cooling process starts at SLAC’s water cooling plant, where nearly 300 tons of chilled water is circulated to the computer center. The water is distributed to the building’s cooling coils, which work like giant radiators in reverse, to extract heat from the air. The cooled air is blown into the 12-inch raised floors of the computer rooms. The current system can cool at a rate of 125 watts per square foot, Weisskopf said, but with a yearly increase in the number of computers installed, an ideal system needs to handle 500-600 watts per square foot.

“We are at the breaking point for old-fashioned under-floor cooling systems,” Weisskopf says. “We’re stuffing thousands more little hot computers in here, and it’s more and more difficult to power and cool them.” Four air handlers, which resemble 14-foot-long giant refrigerators, have been installed to cool areas of the center that produce excessive amounts of heat. Six more are scheduled for installation before winter. But even those won’t be sufficient for long, Weisskopf says. By spring 2006, Weisskopf hopes to install a water-cooling system that will deliver cold water to each individual computer rack in the center.

The ultimate solution is to direct chilled water as close to the computers as possible. Some manufacturers are working on cooling systems that would channel chilled water directly to computer chips. But until the plumbing intricacies are solved, water-cooled racks are the best option for SLAC, Weisskopf says. “If you get a leak [near a computer chip], you’re in trouble,” he says.

Kendra Snyder
Particle physics has been getting its due in the theater world with the recent plays *Copenhagen* and *QED*, which celebrate the lives and work of famous physicists. Now the field is being paid the highest musical and artistic compliment, inspiring the new opera *Doctor Atomic*, which had its première in early October by San Francisco Opera. It tells the story of the Manhattan Project, boiling the action down to a few weeks and hours before the test of the first atomic bomb in April 1945. The opera centers on science director and physicist J. Robert Oppenheimer, his wife Kitty, Edward Teller, General Leslie Groves, and the young idealistic scientist, Robert Wilson. Pulitzer-prize winning composer John Adams wrote the music and his long-time collaborator Peter Sellars directed the opera and cobbled together the libretto from declassified government documents, personal letters, interviews with project participants, and Oppenheimer's favorite poetry.

As a science writer at the Exploratorium, I became involved in this production when the museum was asked by San Francisco Opera to create a companion Web site for the opera, focusing on the scientific, cultural, and historical impact of the atomic bomb. My museum has a stake in the story: physicist Frank Oppenheimer, who founded the Exploratorium in 1969, was the younger brother of J. Robert, and worked alongside him on the Manhattan Project.

So it was with great anticipation that I attended the opera’s première, wondering how the celebrated creators of *Doctor Atomic* would handle such a complex, momentous event in our nation’s history. For the most part, I wasn’t disappointed. It was a musically thrilling, intellectually challenging, and deeply affecting three hours with only a few fizzles. John Adams uses a full palate of musical devices, from electronic compositions that evoke industrial mayhem, to tender passionate duets between Robert and Kitty, to clashing chords and tympani that pulled me to the edge of my seat. The orchestral music was at times full of tension and menace, foreshadowing the bomb detonation and its consequences. At other times, it provided quiet interludes, where the audience could contemplate the legacy of this ultimate weapon of mass destruction. In one of the most gorgeous passages at the end of Act 1, Oppenheimer is alone with his creation, known by scientists as “the gadget,” singing the words of the John Donne sonnet, “Trinity” (for which the bomb test was named): “Batter my heart, three-person’d God.” After fending off his fellow scientists’ moral objections to the bomb’s use against Japan, he surrenders a moment to his own Faustian misgivings.

The libretto was both intriguing and risky. Since Peter Sellars pieced it together from disparate sources and compressed the story into a very short time period, people not familiar with the science or history of the Manhattan Project may feel dropped into the middle of the action with precious little character or plot development. The dialog between physicists was often dense, as when Teller reports that Enrico Fermi was taking bets on whether the bomb test would ignite Earth’s atmosphere in a vast “chain reaction.” (This was an erroneous bit of physics since the question was whether heat from the blast would ignite a thermonuclear fusion reaction, not a fission chain reaction.) For background, it helped to attend the pre-opera lecture and I appreciated that Adams and Sellars never talked down to the audience but assumed we would come to the material with our own knowledge, background, and thoughts about atomic weapons and their use.

Of course, the opera’s dramatic and anticipated high point comes at the end: the bomb goes off. In this age of special effects, Adams and Sellars were subtle. The countdown to the Trinity test stretched out with the orchestra driving relentlessly forward and the chorus shrieking words from the *Bhagavad Gita*: “I am become Death, the destroyer of worlds.” Then all goes quiet, we see the greenish glow of a distant explosion on the faces of the chorus, and then hear the soft voice of a Japanese woman asking for a drink of water—taped testimony from a Hiroshima survivor. Thus, the opera ushers in a new age.

Explore more of *Doctor Atomic* at [www.exploratorium.edu/doctoratomic](http://www.exploratorium.edu/doctoratomic)
Teaching and learning physics in the 21st century

It began with an intense argument. Proponents of one or another viewpoint insisted on evidence and reason. Each side felt that their arguments were sufficient to carry the day. Small groups conferred to reinforce their points of view. But consensus slowly began to emerge as the groups worked throughout the day.

This could describe a gathering of particle physicists collaborating on an experiment or debating the design of the new International Linear Collider. It wasn’t. The participants were teachers at a workshop organized by physicists from Johns Hopkins University. They were exploring data from several cosmic-ray detectors and working to discover the answer to their significant question: “Does the arrival rate of cosmic rays change over a 24-hour day?”

The teachers are part of QuarkNet and were learning about a Web-based electronic laboratory (e-Lab) that uses grid-computing techniques and resources to allow uploading and sharing of data, compiling and executing analysis routines, as well as saving and publishing results. In the classroom, students and teachers from US high schools use the site to investigate scientific questions from simple to complex.

The e-Lab users employ a series of Web forms to select and send their data for analysis. The e-Lab computers push the results back to the user’s Web browser. Users can tweak the analysis by modifying parameters, or show the results to another user for comment. They can even publish an online poster describing their findings. Other users can leave comments on the posters and results.

The e-Lab features a logbook in which users can paste interesting plots or leave notes for later reference. Teachers can look at the logbook entries their students make and leave comments or questions for later consideration. The e-Lab enfolds teaching and learning with the Virtual Data System of the Grid Physics Network (GriPhyn) so that computing jobs or data storage can be supported by the growing resources of the Open Science Grid. For example, data from the cosmic-ray project, like those of most modern physics experiments, require far more computing power and storage capacity than available on classroom computers. The Open Science Grid allows schools to access the resources necessary to do such projects.

QuarkNet has worked with hundreds of physics teachers and physicists since 1999. The program receives funding from the DOE Office of Science and the National Science Foundation. It helps teachers to improve their understanding of science content as well as tools and processes of science.

Five hundred and sixty teachers participate in the program at 53 US institutions. Particle physicists at local universities serve as coaches and mentors. They interact with the teachers in workshops, at their lab benches, and over coffee to talk about new discoveries and ways to help students learn. Both groups of professionals are invested in science; each side can help the other to explore new territory.

Short of having particle accelerators and colliding detectors in each high school, students have little opportunity to collect any evidence that particle physics is as real as the falling apple that demonstrates Newton’s second law of mechanics. QuarkNet enabled many teachers to build cosmic-ray detectors for their classrooms. Scintillating plastic, photomultiplier tubes, readout electronics, and a cheap PC comprise the recipe for a tool that students and teachers can use to explore particle physics in their schools.

Students use these detectors to study cosmic-ray flux, measure muon lifetimes, and search for events simultaneously recorded at several nearby detectors—an indication of extensive showers from highly-energetic cosmic rays. The students must assemble, calibrate, commission, repair, and re-repair their detectors. They must pull cable to the roof so that they can detect GPS satellites for precise timing. They must record which channel on the readout indicates which counter. They must be skeptical about what they observe and explore simple explanations before pronouncing the observation of a new phenomenon. If they believe the observation, they must repeat it—or at least be sure that it was not happenstance.

Sounds familiar? It does to an experimentalist! These intrepid students and teachers are performing the very same tasks as those lucky few who get to crawl over, around, and through the...
massive particle detectors that allow us to peek at the universe in much more interesting conditions than one can find in the local coffee shop. While cosmic-ray events may not contain the same information that Large Hadron Collider events will, they represent an opportunity for students to collect and analyze data in much the same way as modern particle physics collaborations.

These classroom detectors coupled with the grid-enabled e-Lab environment allow students to create engaging experiments, to ask tough questions, and to come closer to doing real science than in most other opportunities for high school students.

Teachers of science—and their students—must understand the true nature of scientific work. They must appreciate that there are few scientists with scientific method posters hanging in their office. (I only know of one, in Fermilab’s Wilson Hall.) Students must realize that science is a field of starts and stops, intensive collaborations, mind-numbing repetition, breathtaking inspiration, and, yes, even politics. Most importantly, students must become adults who can parse a headline like “315 Physicists Report Failure in Search for Supersymmetry” (New York Times, January 5, 1993) and get the true story. QuarkNet’s network of professionals and our exploration of e-Labs will support this understanding, appreciation, and realization.

Tom Jordan

Tom Jordan is a member of the Fermilab Education Office. He is one of five educators who monitor and nurture the QuarkNet program, organize workshops, and visit QuarkNet teachers at their high schools, even sitting in on classroom sessions. He has contributed to the development of the cosmic-ray e-Lab.

For more information about e-Labs, see http://quarknet.fnal.gov/e-labs/
Today’s cutting-edge scientific projects are larger, more complex, and more expensive than ever. Grid computing provides the resources that allow researchers to share knowledge, data, and computer processing power across boundaries. By Katie Yurkewicz

Oliver Gutsche sits in a quiet warren of cubicles in Fermilab’s Wilson Hall, concentrating on his computer screen, ignoring the panoramic view from his 11th-floor window. He’s working feverishly toward a deadline less than two years away, when over 5000 scientists will participate in the largest and most international grid computing experiment ever conducted.

Gutsche is a member of the Compact Muon Solenoid (CMS) particle physics experiment, one of four experiments being built at the Large Hadron Collider at CERN in Switzerland. When the LHC, which will be the world’s highest-energy particle accelerator, begins operating in 2007, vast amounts of data will be collected by its experiments. Scientists worldwide will need to sift through the mountain of data to find elusive evidence of new particles and forces.

“The Compact Muon Solenoid experiment will take 225 megabytes of data each second for a period equivalent to 115 days in 2008,” says Gutsche. “That means each year we’ll collect over two petabytes of data.”

One petabyte is a lot of data (you’d need over 1.4 million CDs to hold it), and the LHC experiments will collect petabytes of data for many years. Any single institution would be hard-pressed to store all that data in one place and provide enough computing power to support thousands of eager scientists needing daily access. Thus the LHC experiments and other scientific collaborations count on a new way to securely share resources: grid computing.
The grid vision
The term grid arose in the late 1990s to describe a computing infrastructure that allows dynamic, distributed collaborations to share resources. Its pioneers envisioned a future where users would access computing resources as needed without worrying about where they came from, much like a person at home now accesses the electric power grid.

One such pioneer, Carl Kesselman from the Information Sciences Institute at the University of Southern California, says, “In today’s society, scientists more often than not operate within an organizational structure that spans many institutes, laboratories, and countries. The grid is about building an information technology infrastructure for such virtual organizations.”

Virtual organizations (VOs) are typically collaborations that span institutional and regional boundaries, change membership frequently, and are governed by a set of rules that define what resources are shared, who is allowed to share them, and the conditions under which sharing occurs. Grids provide the hardware and software that allow VOs to get things done. As cutting-edge scientific tools become larger, more complex, and more expensive, researchers increasingly need access to instruments, data, and collaborators not in their home institution.

“It’s no exaggeration to say that we’ll collect more data in the next five years than we have in all of human history,” says Microsoft’s Tony Hey, former director of the UK e-Science project. “Grid computing and e-Science will allow new, exciting, better-quality science to be done with this deluge of data.”

Applications in many fields
In fields such as biology and geology, grids will enable scientists to bring together vastly different types of data, tools, and research methods to enable scientific breakthroughs.

“For example, there is a group of researchers in England studying the effects of proteins on heart cells,” explains Hey, “and another group in New Zealand with a mechanical model of a heart responding to an electrical stimulus. If the two groups access each other’s data, modeling programs, and computing resources, someday they might be able to determine exactly how a certain protein produced by a genetic defect induces an unusual electrical signal that leads to a heart attack.”

Particle physicists like Gutsche belong to some of the largest scientific collaborations using grids today. Gutsche’s work takes place within the Open Science Grid (OSG), a grid computing project that will provide the framework for US physicists to access LHC data from the ATLAS and CMS experiments. His project is to get a data analysis program running on the OSG, so that the 500 US CMS collaborators can create data sets tailored to their individual research interests. First, however, Gutsche needs to understand the inner workings of grids.

Like many particle physicists, Gutsche’s career requires him to be a part-time computer scientist. Computing expertise, a history of international collaborations, and data-intensive science have led physicists to be founders or early adopters of many distributed computing technologies such as the Internet, the Web, and now grid computing, an application of distributed computing.

“The banking system was an early example of distributed computing,” explains Ian Foster from the University of Chicago and Argonne National Laboratory, who, with Kesselman, published *The Grid: Blueprint for a New Computing Infrastructure*, in 1998. “The system is very focused on moving information around for a very specific purpose using proprietary protocols. In grid computing, there is an emphasis on bringing together distributed resources for a variety of purposes using open protocols.”

How grids work
Grids will enable scientists, and the public, to use resources, access information, and connect to people in ways that aren’t possible now. A unified grid-computing
A system that links people with resources is made up of four layers of resources and software stacked on top of each other. Each layer of this grid architecture depends on those below it. The network layer is at the base. It connects all of the grid's resources, which make up the second layer. On top of the resources sits the middleware, the software that makes the grid work and hides its complexity from the grid user. Most people will eventually only interact with the uppermost software layer, the applications, which is the most diverse layer. It includes any program someone wants to run using grid resources.

Using the grid, a scientist could sit down at her computer and request, for example, a climate prediction for the next 10 years. She would open the appropriate grid-adapted application and provide the geographic location as well as the time range for the prediction. The application and middleware will do the rest: make sure she's a member of a VO that allows her to access climate resources; locate the necessary historical data; run a climate prediction program on available resources; and return the results to her local computer.

The steps that have been taken so far toward the seamless grid vision have been made possible by a sudden increase in network connectivity over the last decade.

"Companies had installed a lot of optical fiber, thinking they'd be able to sell it at a good profit," says Stanford Linear Accelerator Center’s Les Cottrell. "When the bubble burst, instead of selling it to other companies at a fire-sale rate, many of the businesses were willing to negotiate deals with academic and research organizations. As a result, for example, the SLAC connection to the Internet backbone has increased over 60 times since 2000, from 155 megabits per second to 10 gigabits per second, and we can send ten times as much data across trans-Atlantic lines in the same amount of time."

The availability of better network hardware, software, and management tools allows scientists to use the grid to share more than just processing power or files. The resource layer of the grid, connected by high-speed networks, also includes data storage, databases, software repositories, and even potentially sensors like telescopes, microscopes, and weather balloons.

Where’s my grid?

Many members of large science collaborations already have specialized grids available to advance their research. Those not so fortunate may well have access to shared resources through one of the many multidisciplinary projects sprouting up worldwide. These grids range from “test beds” of only a few computers to fully-fledged projects sharing vast resources across continents.

University researchers and students use campus grids, such as the Grid Laboratory of Wisconsin (GLOW) at the University of Wisconsin-Madison, or the Nanyang Campus Grid in Singapore, to share computing resources from different departments. Universities that haven’t caught the grid bug yet can join state-wide or regional projects such as the North Carolina Statewide Grid, which will benefit business, academia, and government when completed, or SEE-Grid, which includes 10 countries in south-eastern Europe.

National grid computing projects abound. In Japan, researchers in academia and business use NAREGI, and over 25 European countries have access to either a national grid or to the European Union-funded Enabling Grids in E-science (EGEE) infrastructure. In the United States, collaborations can share and access resources using the Open Science Grid (OSG) infrastructure, or apply for time on the TeraGrid, which links high-end computing, storage, and visualization resources through a dedicated network.

The brains of a grid

Making many different networks and resources look like a unified resource is the job of the middleware—the “brains” of a grid. The types of middleware used by a grid depend on the project’s purpose.

“If you’re building an information grid, where you’re collecting information from 15,000 radio antennas, you focus on information services,” explains Olle Mulmo from the Royal Institute of Technology in Sweden. “If you’re making lots of CPUs..."
available, you focus on resource management services. You'll need data services if you're compiling a lot of data and making it available to others. The fourth main category is security, which works across all other categories.

Enforcing a VO's rules about who can access which resources, making sure that access is secure, and keeping track of who is doing what on a grid creates some of the most challenging problems for grid developers. The middleware must provide the solutions.

"Without security--authorization, authentication, and accounting--there is no grid," explains Fabrizio Gagliardi, project director for the Enabling Grids for E-sciencE project funded by the European Union.

The stringent requirements for security and accounting differentiate grid computing from other distributed computing applications. Advances in security already allow academic researchers to use grid technology, but many obstacles remain to grids' commercial use.

"In particle physics, once you've verified that you belong to a certain VO, it doesn't really matter which of the VO's resources you use," adds Gagliardi. "But if you're submitting grid jobs to a business that's charging for resources, there must be a strict accounting of which resources you've used and how much you've used them."

**A myriad of grids**

Gutsche is adapting a CMS analysis application that already runs on the LHC Computing Grid (LCG), the infrastructure that supports European LHC physicists, to run on the US-based OSG. Due to differences in middleware, the same application doesn't automatically run on both the LCG and the OSG. This is common in today's grid world, which includes small, large, single-focus, and multi-disciplinary grids.

Right now, a grid expert will spend weeks or months adapting a certain application to interface with one flavor of grid middleware, and then repeat the process to use another grid. Once standards have been adopted by the grid community, making applications work on one or more grids will be much easier.

"The grid community is now big enough and experienced enough that users may need to talk to several grid infrastructures," says Mulmo. "To do that today, they often have to have several middlewares installed. But now we start to see the international communities and collaborations forcing us--the middleware developers--to cooperate on common interfaces and interoperability."

Grid visionaries believe that, eventually, there will be one worldwide "Grid" made up of many smaller grids that operate seamlessly.

"It's always going to be a bit like the Internet," says Foster, "with common protocols, and a lot of common software, but lots of different networks designed to deliver a different quality of service to different communities. Some large communities will want or need their own dedicated infrastructure, but the small group of archaeologists will need to use general-purpose infrastructures."

**First signs of success**

Gutsche sits at his computer and prepares to test the data analysis application on the grid. He initializes his grid interface and goes through the steps to identify himself to the OSG and the LCG. The program will extract statistics from a particle physics data set. He selects the data set he wants from a Web site, and types the names of both the data set and the program into a small file. He starts the user analysis submission application, which reads the file. The computer takes it from here. It splits the request into many smaller jobs and submits them to a central computer known as the resource broker.

The resource broker finds the data set, makes sure it is complete, and checks the computer farm where the data is located to verify that there are enough resources to run all of Gutsche's jobs. If so, his requests are scheduled on the farm. If all goes well the jobs will run successfully and Gutsche can collect the results from the resource broker.
Grid growth will drive supercomputing capacities

The growth of grid computing could super-size the future of supercomputers, if Horst Simon is on the mark. “There are some who think that supercomputing could be replaced by the grid,” says Simon, of the National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory. “For example, using many PCs, SETI@home is a clear success, and it can do a significant job.

“But I use the analogy of the electric power grid,” Simon continues. “It would be great to have a lot of windmills and solar panels producing electricity across the whole country, but now, we still can’t run the power grid without the large power plants. In the same way, supercomputers are truly the power plants to drive the computing that cannot be distributed across the grid.

“So the grid will drive even more demand for supercomputing, which can produce more and more data to effectively utilize the capacity of grid computing. Think of the LHC and the Tevatron as supercomputers—grid computing will support CMS, ATLAS, all the particle physics detectors as the accelerator-supercomputers produce more and more data.”

Simon and colleagues Hans Meuer, of the University of Mannheim, Germany; Erich Strohmaier, of NERSC; and Jack Dongarra, of the University of Tennessee-Knoxville, produce the twice-yearly Top500 list of the world’s fastest supercomputers. Their next list will be published at SC05 in Seattle, November 12-18, the annual international conference on high performance computing, networking and storage. On the current list, which was released at the ISC2005 conference in Heidelberg, Germany, on June 22, the top spot went to the BlueGene/L System, a joint development of IBM and DOE’s National Nuclear Security Administration (NNSA) and installed at DOE’s Lawrence Livermore National Laboratory. BlueGene hit 136.8 teraflops, or trillions of calculations, per second, although Simon granted that judging a supercomputer solely on speed is like judging a particle accelerator solely on brightness.

The definition of a supercomputer has evolved since the Top500 list originated in 1993, due to the competitive performance of massively parallel technologies in the 1990s. Now, supercomputers are defined as the largest systems available at any given time for solving the most important problems in science and engineering, although they are primarily used for science applications. Simon sees a growth spiral for supercomputing-grid synergy. “Supercomputing and the grid are complimentary—mutually reinforcing,” he says. “The grid provides the right tools in the middleware to get more science out of the data.”

Just before stopping for lunch, Gutsche receives an instant message from a CMS researcher who wants help analyzing data on the grid. This is one of the first requests Gutsche has received, and he knows that it won’t be the last one. Grids are catching on, and Gutsche looks forward to helping more and more people get started, watching grids grow into standard tools for great discoveries.
All fields of science benefit from more resources and better collaboration, so it’s no surprise that scientific researchers are among the first to explore the potential of grid computing to connect people, tools, and technology. Physics and biology were among the earliest adopters, but chemistry, astronomy, the geosciences, medicine, engineering, and even social and environmental sciences are now kick-starting their own efforts. Here is a small sampling of some of the projects now pushing the limits of grid computing.

by Katie Yurkewicz
Identifying Alzheimer’s disease before a person exhibits symptoms; learning the function of all the genes in the human genome; finding drugs to cure and prevent malaria: From large dedicated biomedical infrastructures to small individual applications, grid computing aids scientists in their quest to solve these and other biological, medical, and health science problems.

One of the first, and largest, of the dedicated cyberinfrastructures is the Biomedical Informatics Research Network (BIRN). Launched in 2001, the National Institutes of Health-funded project encourages collaboration among scientists who traditionally conducted independent investigations. BIRN provides a framework in which researchers pool data, patient populations, visualization tools, as well as analysis and modeling software.

In one of BIRN’s three test beds, magnetic-resonance images from small groups across the country are pooled to form a large population for the study of depression, Alzheimer’s disease, and cognitive impairment. A large group of subjects makes for a very comprehensive study, but comparing MRI scans taken at different institutions is a challenge worthy of grid computing.

“If you gave several people different cameras from different makers and asked them to take the same picture, they’d all come out a little different,” explains Mark Ellisman, director of the BIRN Coordinating Center at the San Diego Supercomputer Center. “If you want to search MRI images for small structural differences in the brains of patients with Alzheimer’s disease, you need to make the data from all the MRI machines comparable. This requires methods to align, measure, analyze, and visualize many different types of data, which researchers can develop and share using the BIRN framework.”

While BIRN brings together hundreds of scientists in a dedicated infrastructure, a handful of scientists in France are grid-adapting an application to increase the accuracy of cancer treatment.

Medical physicists planning radiation therapy treatment must simulate the passage of ionizing radiation through the body. GATE, the GEANT4 Application for Tomographic Emission, provides a more accurate method for such simulations than many existing programs, but its long running time makes it inefficient for clinical settings. By running in the Enabling Grids for E-sciencE (EGEE) infrastructure, researchers have decreased by a factor of 30 GATE’s running time. Medical physicists at the Centre Jean-Perrin hospital in France are now testing the use of GATE and EGEE to increase the accuracy of the treatment of eye tumors.

“Without the resources shared on EGEE, one simulation would take over four hours to run,” says graduate student Lydia Maigne, who has adapted GATE to work on the grid. “When split up into 100 jobs and run on the grid, it only takes about eight minutes.”

In the field of genomics, the amount of data available has exploded in recent years, making the analysis of genome and protein sequences a prime candidate for the use of grid resources. Computer scientists and biologists at Argonne National Laboratory have developed a bioinformatics application to interpret newly-sequenced genomes. The Genome Analysis and Database Update system (GADU), which runs on the Genome Analysis Research Environment, uses resources on the Open Science Grid and the TeraGrid simultaneously to compare individual protein sequences against all annotated sequences in publicly available databases.

Every few months, researchers run GADU to search the huge protein databases for new additions, and compare the new proteins against all those whose functions are already known. The use of grid computing has greatly reduced the time for a full update, which had skyrocketed due to the exponential increase in the number of sequenced proteins.

Mouse BIRN researchers are using multi-scale imaging methods to characterize mouse models of human neurological disorders.

Image: Diana Price and Eliezer Masliah, Mouse BIRN
A comprehensive understanding of the Earth’s evolution over time, or of the effect of natural disasters on geology and human-made structures, can only be achieved by pooling the knowledge of scientists and engineers from many different sub-specialties. Two US experiments are examples of how the geoscience and earthquake engineering communities are exploring grid computing as a tool to create an environment where sharing of ideas, data, as well as modeling and visualization resources are commonplace.

The researchers of the Geosciences Network (GEON) are driven by their quest to understand quantitatively the evolution of the North American lithosphere, or Earth’s crust, over space and time. GEON will integrate, and make accessible to the whole community, data and resources currently accessible to only a few experts. Tools currently under development, like smart search technology, will allow scientists looking for information outside their specialties to find what they need without knowing too much information about a specific data set or database.

“The Earth is one unified system,” says geophysicist Dogan Seber, GEON project manager. “To really understand it, we need an infrastructure that any of us can easily use to extract information and resources from other disciplines. My interest is intracontinental mountains, and using geophysics I can understand only some aspects of the system. To understand the whole thing—how they started, why they started, what’s happened over time—I also need to know about sedimentation, tectonics, and geologic history.”

The George E. Brown, Jr. Network for Earthquake Engineering Simulation (NEES) seeks to lessen the impact of earthquake-and tsunami-related disasters by providing revolutionary capabilities for earthquake engineering research. Its cyberinfrastructure center, NEESit, uses networking and grid-computing technologies to link researchers with resources and equipment, allowing distributed teams to plan, perform, and publish experiments at 15 NEES laboratories across the country.

NEESit researchers develop telepresence tools that stream and synchronize all types of data, so that key researchers can make informed decisions during an experiment even if they’re sitting thousands of miles away. After the experiment, researchers will upload data to a central data repository, access related data, and use portals to simulate, model, and analyze the results.

“Scientists can or will participate remotely in experiments, such as tests of wall-type structures, at the University of Minnesota; long-span bridges, at the University of Buffalo; or the effect of tsunamis using a wave basin, at Oregon State,” says Lelli Van Den Einde, assistant director for NEESit Operations. “Our goal is that researchers will upload their data soon after a test has occurred, and once the data have been published they will be made available to the public.”

Both GEON and NEES began as US experiments and are funded by the National Science Foundation, but they are making an impact worldwide. Researchers in Korea are developing their own version of NEES, and through GEON, countries in South America and Asia are discovering how to use grid technology to understand the Earth.
While biomedicine and geoscience use grids to bring together many different sub-disciplines, particle physicists use grid computing to increase computing power and storage resources, and to access and analyze vast amounts of data collected from detectors at the world’s most powerful accelerators.

Particle physics detectors generate mountains of data, and even more must be simulated to interpret it. The upcoming experiments at CERN’s Large Hadron Collider—ALICE, ATLAS, CMS, and LHCb—will rely on grid computing to distribute data to collaborators around the world, and to provide a unified environment for physicists to analyze data on their laptops, local computer clusters, or grid resources on the other side of the globe.

“When data become available from the ATLAS detector, we will want to sift through it to find the parts relevant to our research area,” says Jim Shank, executive project manager for US ATLAS Software and Computing. “The data sets will be too large to fit on users’ own computing resources, so they will have to search through and analyze events using grid resources. We are now dedicating a lot of manpower to building a system that will allow physicists to access the data as easily as if they were working at CERN.”

While the LHC experiments might be making more headlines recently, Fermilab’s DZero experiment has used grid computing to reprocess one billion events over the past six months. DZero has a long history of using computing resources from outside Fermilab, and since 2004 has been using the SAMgrid to create a unified computing environment for reprocessing and simulation.

The reprocessing of stored data is necessary when physicists have made significant advances in understanding a detector and computer scientists have optimized the software to process each collision event more quickly. With the DZero resources at Fermilab busy processing new data constantly streaming in, the collaboration has to use outside resources for the reprocessing.

“The reprocessed data has a better understanding of the DZero detector, which allows us to make more precise measurements of known particles and forces, and to better our searches for new phenomena,” explains Fermilab’s Amber Boehnlein. “We never would have been able to do this with only Fermilab resources.”

With the reprocessing successfully completed, DZero researchers will now use SAMgrid for Monte Carlo simulations of events in their detector. Monte Carlo programs are used to simulate a detector’s response to a certain type of particle, such as a top or bottom quark. Without simulated data, physicists could make no measurements or discoveries. Thus, all particle physics experiments generate vast numbers of Monte Carlo simulations. Many—including DZero, ATLAS, CMS, and BaBar at SLAC—have turned to grids for help.

“US CMS has been using grid tools to run our Monte Carlo simulations for over two years,” says Lothar Bauerdick, head of US CMS Software and Computing. “It’s much easier to run simulations than analysis on the grid, because simulations can be split up into many smaller identical pieces, shipped out across the grid to run, and brought back together in a central place.”

Physicists on the LHC experiments, and those looking to build even larger and more data-intensive experiments in the future, hope that the success of the grid for Monte Carlo simulation will be replicated for data analysis, enabling scientists to gain a greater understanding of the universe’s fundamental particles.
You go to a home supplies store and purchase the oak board for those shelves you need to add to your basement. You haul it home and discover integrated within the wood are instructions for building not just the bookcase but your entire basement redesign, along with all the tools you’ll need—and the expertise to use them, plus a support group standing by to offer help and suggestions while you cut and drill, hammer and fit.

This do-it-yourself fantasy is not far removed from the way physicists are now working on facilities that include one of the biggest projects ever mounted in science: the development of the proposed International Linear Collider. Serving as combination instruction manual/toolkit/support network is **GEANT4**, a freely-available software package that simulates the passage of particles through scientific instruments, based on the laws of particles interacting with matter and forces, across a wide energy range. Besides its critical use in high-energy physics (its initial purpose) **GEANT4** has also been applied to nuclear experiments, and to accelerator, space, and medical physics studies.
The effects of the radiation environment on the instruments of the XMM-Newton spacecraft were modeled with G4Ant4 prior to launch by the European Space Agency in 1999. XMM-Newton carries the most sensitive X-ray telescope ever built.

Illustration: ESA-Ducros

Left Photo: A GEANT4 visualization of the CMS detector, which weighs in at nearly 14,000 tons. During one second of CMS running, a data volume equivalent to 10,000 copies of the Encyclopaedia Britannica is recorded.

Image: CMS collaboration

Right Image: GEANT4 simulation of a supersymmetry event (showing leptons and missing transverse energy), with a Higgs particle decaying to two Z particles and to four muons in the full Compact Muon Solenoid detector.

Image: CMS collaboration
“The benefit that has struck me most strongly is the way geant4 can be used to help in treating tumors,” says Fermilab’s Daniel Elvira. The European Particle Physics Laboratory (CERN) and Stanford Linear Accelerator Center (SLAC) are the focal points of geant4 resources; Elvira heads up a small but growing geant4 team at Fermilab, providing support for individual users and experiment collaborations at the lab. He continues: “This is a very nice example how a physics-based tool, developed in a physics environment, has filtered to other communities in such effective ways. Simulations are now used in all places in society. Simulations enable the optimization of designs for better performance with lower costs, in the same way that the Internet saves money through the sharing of information."

Building with objects

geant4 is “object-oriented” in design and function. A segment of data (an “object”) is encapsulated with the routines or methods that operate on that data. In other words, the information knows how to process itself when a user retrieves it. Almost by definition, geant4 can handle virtually any simulation task within reasonable bounds; maybe even within unreasonable bounds.

“Practically everything is an object—a detector, a particle, a particle track, a vertex, a hit in the detectors,” says Fermilab’s Maya Stavrianakou, working with geant4 at CERN in the completion stages of the Compact Muon Solenoid detector for the Large Hadron Collider.

The complex CMS detector has about 100 million events used for physics preparation studies. The attributes and interactions of a dynamic particle in the detector can be described and retrieved in geant4—with all requisite tools and operations attached.

GEANT4 heritage

As with any tool so valuable and easy to use, geant4 (from “Geometry and Tracking”) was years in the making—decades, in fact. It also embodies the transition of scientific computing code from the programming language fortran (“formula translation”), developed by IBM in the 1950s, to C++, the object-oriented language developed in the 1980s. C++ grew from the C language developed in the 1970s at Bell Labs for the UNIX operating system. Ancestors of geant4 software written in fortran date back to CERN experiments in the 1980s at the Large Electron-Positron collider, but the specific genesis of geant4—the current indispensable package—springs from a 1994 proposal to the CERN Detector Research and Development Committee, for rewriting the software code into C++. The proposal was approved as RD44, reporting to the CERN Large Hadron Collider Committee.

But geant4 is an ongoing worldwide collaboration as much as it is a software package with worldwide use. The software from its beginnings was an independent project, developed through the efforts of more than 100 scientists from more than 40 institutes and experiments in Europe, Russia, Japan, Canada, and the United States, all signatories to a Memorandum of Understanding that is renewed every two years. Governance is through a Collaboration Board (CB), a Technical Steering Board, and several working groups. The Technical Steering Board, chaired by CERN’s John Apostolakis, is judge and jury for software and physics issues, for user requests, and for suggested software revisions. Responsibilities of the Collaboration Board, chaired by SLAC’s Richard Mount, include monitoring the overall allocation of resources.

“The CB consists, in the main, of people with the power to allocate resources within their institution,” Mount explains. “When resource-related issues are brought to the CB, it allows institutional decisions to be made on the basis of a full knowledge of what geant4 needs, and what is likely to be available from other parts of the collaboration.”

GEANT4 and ILC

geant4 is being used to design three International Linear Collider detector concepts by three interdependent global collaborations. “The software used in this design process must provide full simulation capabilities for the whole International Linear Collider physics program, including physics simulations, detector designs, and machine backgrounds,” says Norman Graf of SLAC, leader of the North American Detector simulation group. “The goal is to have a common simulation environment used in all ILC studies which allows sharing of detectors, algorithms, and code. The system should be flexible, powerful, yet simple to install and maintain.”

GEANT4 is being used to design highly efficient detectors to explore the physics from events produced at the ILC, such as this simulated response to \( e^+ e^- \rightarrow Z (\rightarrow \mu^+ \mu^-) + higgs (\rightarrow b\bar{b}) \)

Image: Norman Graf
A detector design must begin somewhere; usually, it begins with the physics motivation and just the barest sketch of a detector. Momentum, angular resolution, and angular acceptance are the crucial parameters. Monte Carlo simulations of particle interactions generate the physics analysis of what will occur inside the detector.

“Since the desired precision and performance of the ILC detectors has to be much higher than in previous general purpose collider detectors,” Graf says, “we have adopted an approach which allows many detectors to be quickly simulated at a reasonable level. We would only proceed to very detailed designs once an overall optimum has been determined. We can also simulate subdetector prototypes which are built as part of the detector R&D process. This allows a seamless integration of test beam results into the simulation process.”

**GEANT4 in space**

Both NASA and the European Space Agency have benefited from GEANT4 applications in spacecraft design, notably in ESA’s Newton spacecraft and NASA’s Gamma Ray Large Area Space Telescope (GLAST), a joint project with the US Department of Energy and with agencies in France, Italy, Japan, and Sweden. GLAST will detect gamma rays—high-energy photons—from the central regions of exotic objects like supermassive black holes, pulsars, and gamma-ray bursts. The projected launch is August 2007.

The GLAST Large Area Telescope has four main components: a precision tracker, based on silicon-strip detectors; a calorimeter, using cesium-iodide bars to measure the energy of the cosmic ray particles; a data acquisition system, with 32-bit radiation-hard processors; and an anticoincidence detector to discount the high-energy cosmic-ray background. For all practical purposes, GLAST is a high-energy-physics particle detector in space, and GEANT4 simulations have been on the job in exploring the radiation environment.

“Because of the very reliable electromagnetic simulations, we use GEANT4 to simulate our photon signals and to explore how hadrons might sneak into the detector through cracks or through the bottom and try to look like photons,” says Richard Dubois of SLAC. “We require good EM simulation from a few MeV up to hundreds of GeV.”

**GEANT4 in medicine**

SLAC has become a major US collaborator for medical physicists working on GEANT4 applications, particularly in hadron therapy and brachytherapy for the treatment of tumors. Hadron therapy uses external beams of heavy particles (such as protons) and ions (such as carbon) for cancer treatment—a procedure first suggested by Fermilab founding director Robert Rathbun Wilson in 1946 in his paper, “Radiological use of fast protons,” published in *Radiobiology*. Brachytherapy implants a radiation source close to a cancer, using tubes or catheters. GEANT4 can simulate a typical hadron-therapy treatment beam line and calculate the proton/ion dose distribution curves. It can also calculate the depth-dose distribution in a given material, and illustrate the most effective use of the beam in hadron therapy.

Joseph Perl heads up the effort on medical applications of GEANT4 at SLAC, offering expertise to medical researchers at nearby institutions such as University of California, San Francisco; University of California, Santa Cruz; and Stanford University Medical Center; and working with colleagues at KEK in Japan to develop additional tools to aid medical researchers, such as easy-to-reuse simulations of standard medical-physics dose detectors. Perl has also played a leading role in organizing the GEANT4 North American Medical Users Organization (G4NAMU), launched in May of 2005. G4NAMU brings together the GEANT4 medical user community in North America, to share issues and advice, develop regional collaboration, and communicate as a group with GEANT4 developers. The first major meeting, in July 2005, took place at the annual meeting of the American Association of Physicists in Medicine in Seattle.

“SLAC has one of the largest concentrations in the world of GEANT4 expertise,” says Perl, “comprising experts in all parts of GEANT4 from hadronics and electromagnetics to software kernel, user interface, visualization, and documentation. But the real expertise in medical applications lies with the medical physicists who work in smaller groups throughout the world. Our intention from SLAC is not to replicate that expertise but rather to refine the GEANT4 toolkit to better serve those experts.”

**Take it to the limits**

Solving problems, visualizing complex environments, saving time, saving effort, saving money—how far could GEANT4 take all these advantages? Not as far as making a discovery, Elvira says.

“Simulations are an essential part of the work, but they cannot teach us physics that we do not know,” he says. “We can learn how to search for particles that have certain properties predicted by theorists; for example, the properties of the Higgs boson. But we cannot learn about the properties of new or undiscovered particles through simulations. We cannot replace the experiments. We will always need the experiments.”
A piece of steel may look cold and lifeless. But like any other piece of matter, it is bursting with activity deep inside. Electrons whiz around inside atoms, and a sea of never-resting quarks and gluons populates the nucleons that make up the atomic core.
For more than 30 years, researchers have tried to get a handle on how the quarks clump under the influence of the strong force to form protons and other constituents of matter. Although theorists discovered quantum chromodynamics (QCD)—the set of equations that describe the strong force—in the early 1970s, solving the equations has always been a struggle. The calculation of particle processes at low energy seemed impenetrable, and results produced by crude approximations didn’t match experimenters’ observations.

That has changed. During the last two years, the perseverance in taming the equations of QCD with supercomputing power has finally begun to pay off. Using ever-more-sophisticated computers and algorithms, theorists have begun to reproduce experimental results for QCD phenomena such as the decay of a quark-antiquark pair at rest. Moreover, in the last twelve months theorists took the lead and predicted physical quantities. To the theorists’ delight, new experimental results then matched the theoretical numbers with equal precision.

“To do the necessary calculations has proved very challenging, and the only technique that has really succeeded is to directly ‘discretize’ the equations, feed them into a computer, and let the computer work very hard,” explained Frank Wilczek when receiving the Nobel Prize in Physics in 2004, which we shared with David Gross and David Politzer. “In fact, these kinds of calculations have pushed the frontiers of massively parallel computer processing.”

**Quantum rubber bands**

Gross, Politzer, and Wilczek discovered in 1973 that the strong force between two quarks is rather weak when the quarks are close together—a phenomenon called asymptotic freedom. But as the distance increases, the strong force—mediated by gluons—acts like a rubber band strong enough to prevent, say, a single quark from escaping the interior of a proton. Even when the rubber band “snaps,” no single quark is produced. Instead, following Einstein’s equation $E=mc^2$, the energy released creates two extra quarks that take the place of the free ends of the broken rubber band halves.

“Experimentalists don’t observe free quarks,” says Fermilab’s Andreas Kronfeld, who is an expert in QCD calculations using computers. “To measure and understand quark properties, you need theorists to relate quarks to what is observed in experiments. The tool to use to get to the quark interactions is lattice QCD.”

In quantum theories such as QCD, particles are represented by fields. To simulate the quark and gluon activities inside matter on a computer, theorists calculate the evolution of the fields on a four-dimensional lattice representing space and time. Using today’s computers, a typical lattice simulation that approximates a volume containing a proton might use a grid of 24×24×24 points in space evaluated over a sequence of 48 points in time. The values at the intersections of the lattice approximate the local strength of quark fields. The links between the points simulate the rubber bands—the strength of the gluon fields that carry energy and other properties of the strong force through space and time, manipulating the quark fields.

At each step in time, the computer recalculates the field strengths at each point and link in space. In its simplest form, the algorithm for a single point takes into account the changing fields at the eight nearest-neighbor points, representing the exchange of gluons in three directions of space—up and down; left and right; front and back—and the change of the fields over time—past and future. Starting with random quark and gluon fields, theorists...
produce hundreds of configurations that are the basis for calculating properties such as the masses of particles composed of quarks.

“Lattice QCD is a solid, predictive theory,” says Kronfeld. “However, you have a finite but huge number of integrals to do. And that’s what has taken us so long.”

**Teraflops for QCD**

The computing power needed for these calculations is immense. Since the invention of lattice QCD by Kenneth Wilson in 1974, theoretical physicists have sought access to the most powerful computers, and physicists have actively contributed to the development of high-performance parallel computers. In the 1980s, the Cosmic Cube machines at Caltech, the Columbia University computers, the GF11 project at IBM, the Italian APE computers, the Fermilab ACPMAPS installation and the PACS machines in Japan were all designed and built out of the desire to simulate lattice QCD.

While the performance of the early machines was still measured in megaflops (one million floating point operations per second), the computing power reached tens of gigaflops in the early 1990s. Today’s top-performance computers for the lattice QCD community—the QCD-on-a-chip (QCDOC) machines developed by a US-Japan-UK collaboration, and the next-generation machines of the Array Processor Experiment (apeNEXT) in Europe—operate in the multi-teraflops (millions of megaflops) range. A 1.2-teraflop machine, the SR8000F1 supercomputer at KEK, will be replaced with a more powerful machine in 2006. Using an alternative approach, scientists at Fermilab and Thomas Jefferson National Laboratory (JLab) hope to achieve over two teraflops for lattice QCD applications with large clusters of off-the-shelf PCs this spring.

The US lattice QCD program, which includes approximately 200 scientists, is supported by the Department of Energy and the National Science Foundation. The scientific activities of the program are coordinated by a national lattice QCD executive committee.

“Our job is to lead the efforts to construct the infrastructure,” says committee chairman Bob Sugar, of the University of California, Santa Barbara. “We determine what hardware and software best meets the needs of the field. We draw plans, raise money, and see that the plans are properly implemented.”

Three factors play the primary roles in determining the performance of a massively parallel computer: the rate at which the central processing unit (CPU) performs floating point operations (additions and multiplications); the
rate at which data is transferred between the processor’s memory and its CPU; and the rate at which data is transferred between processors. The optimal balance among these three rates depends strongly on the problem being studied.

Commercial supercomputers, which must perform well on a wide variety of problems, are generally not optimal for any particular one. However, a computer designed for a single problem balances the CPU speed and data movement rates to optimize total performance and price-to-performance ratio. For this reason, lattice QCD scientists around the world increasingly build their own computers, obtaining significantly better price/performance than with commercial supercomputers.

The QCDOC and apeNEXT collaborations have taken the custom design of QCD machines to the next level. Scientists in these groups designed custom microchips that integrate a microprocessor unit, memory, and network communication interfaces as well as several megabytes of on-chip memory, an approach known as System-on-a-Chip (SoC) design.

“The communication of a microprocessor with memory is terribly complicated,” says apeNEXT collaborator Hubert Simma, a physicist at the German laboratory DESY Zeuthen. “Normally, you use a separate microchip to handle this communication, which increases the time it takes to access data. By integrating the memory and networking interfaces on the same chip as the processor, you achieve much faster access.”

The compact design of the QCDOC and apeNEXT machines reduces the physical size of these supercomputers and their consumption of electrical power, thereby reducing the need for cooling—a major concern for most commercial supercomputers. A typical supercomputer might consume many thousand kilowatts of power, producing the same amount of heat as tens of thousands of light bulbs. In contrast, a QCDOC machine, which has 12,288 microprocessors and a peak performance of 10 teraflops, requires only about 100 kilowatts of power, greatly reducing its cost of operation. The apeNEXT computers have racks with 512 microprocessors and a peak performance of 0.66 teraflops, and seven of 24 racks have been built so far. The racks will be distributed among INFN Rome (12), DESY Zeuthen (4), Universität Bielefeld (6) and Université de Paris-Sud (2).

**Cooperating with industry**

Designing and building QCD supercomputers often happens in close connection with industry. Japanese lattice QCD scientists, for example, have worked with the supercomputer company Hitachi in the past. And the microchips of the apeNEXT machines “represent one of the few cases of complete computing processors developed in Europe,” says Raffaele Tripiccione, coordinator of the apeNEXT project. Its chip design is the basis for the 1-gigaflops-plus mAgic processor, produced by Atmel, a company with headquarters in California. In contrast to other high-performance chips, the mAgic architecture delivers its performance at a low clock frequency of 100 MHz, lowering power consumption and heat dissipation in the same way as the apeNEXT and QCDOC machines.

The QCDOC collaboration built on more than 20 years of experience in QCD supercomputer design at Columbia University, under the visionary leadership of Norman Christ; the collaboration worked closely with experts from IBM’s Thomas J. Watson Research Center, which developed its own QCD machine, GF11, in the late 80s and early 90s. Other collaboration members came from Brookhaven National Laboratory, the RIKEN BNL Research Center, and the University of Edinburgh. The $15-million cost for the construction of three QCDOC machines was shared equally among the US Department of
Energy, RIKEN (the Institute Physical and Chemical Research in Japan), and the Particle Physics and Astrophysics Research Council (PPARC) in the United Kingdom. For the DOE computer, assigning computer time to various QCD projects is the task of the Lattice QCD Executive Committee.

No.1 in the TOP500
The exceptional price-to-performance ratio of the QCDOC project, which cost approximately $1 per megaflop, as well as the low power consumption of the QCDOC machines, make it the choice for the foundation of a new generation of IBM supercomputers known as BlueGene/L. To make the new supercomputer more attractive for a broad class of applications, IBM generalized the massively parallel QCDOC architecture while retaining its cost and power-consumption advantages. The modest performance of the BlueGene SoC processors is offset by the fact that more than one thousand processors fit into a single rack without exceeding standard cooling capabilities.

The largest BlueGene/L machine built to date is a supercomputer with 65536 processors, which is currently listed as No.1 in the TOP500 list of supercomputers. It achieves a performance of 136.8 teraflops on the benchmark used for the TOP500 listing, but the performance on QCD code would be significantly lower.

“BlueGene is the son of QCDOC,” says Nicholas Samios with pride. Samios is the director of the RIKEN BNL Research Center, a RIKEN sister institute located at BNL. “IBM was involved in the R&D [of the QCDOC machine] from the very beginning.”

In fact, the BlueGene supercomputer has retained enough of the QCDOC characteristics that the machine is still a viable QCD machine. According to Shoji Hashimoto, scientist at the Japanese particle physics laboratory KEK, his lab will begin operating a Blue Gene machine with a peak performance of 57.3 teraflops in March 2006, using it for lattice QCD and other applications. For QCD code, the machine is expected to sustain 12 to 15 teraflops.

The demand for more powerful QCD machines also persists in the United States. “We are having scheduling problems,” says Samios about the RIKEN machine. “I think ten teraflops does not satisfy the appetite of these people. Our scientists are very imaginative. When they have more computing power, they find things to do that they couldn't do before.”

PC clusters
The Department of Energy is also funding an alternative approach to providing the lattice QCD community with enough computing power at low cost. Instead of building special-purpose machines, scientists at Fermilab and JLab are taking advantage of powerful and low-cost off-the-shelf computer components, building large, sophisticated PC clusters dedicated to QCD simulations.

The idea goes back to the mid-90s, when Fermilab began using PC clusters for the computing-intensive analysis of large amounts of experimental data. In late 1997, Don Holmgren, who helped to set up the first PC clusters, was looking for additional applications. He approached Fermilab theorist Paul Mackenzie, who now serves on the Lattice QCD Executive Committee.

“We were trying to do this revolution,” says Holmgren. “At the time, PCs and Linux machines were much more cost effective for the processing of the huge amount of data collected by the particle physics experiments. So we asked around and looked for other applications.”

To test the idea, Holmgren and Mackenzie built the first small cluster for QCD applications in 1999. In 2001, the DOE Scientific Discovery through Advanced Computing (SciDAC) program began to provide funding to Fermilab and JLab to build clusters for the lattice QCD community. The clusters have
grown in size, and every year the labs buy the best PCs and networking technology, eventually discarding the old systems. Today, Fermilab operates three clusters with a total of 512 PCs with Intel Xeon and Pentium processors, and Myrinet and Infiniband networking technologies. JLab owns three clusters with a total of 768 Intel Xeon processors using Myrinet and gigabit ethernet mesh networks. Together, the Fermilab and JLab clusters sustain about 1.3 teraflops on QCD code. In connection with the purpose-built QCD machines, PC clusters provide theorists with a range of computing power for different types of QCD calculations.

For PC clusters, communication among processors is as important as for QCD supercomputers. For a prototype system built in 2000, Fermilab spent as much money on the communication network as on the 80 PCs themselves. Although PC clusters are limited in size due to power consumption, space constraints, and scalability of off-the-shelf components, they are a cost-effective solution that allows for annual upgrades with the latest PC technology. Over the next four years, the DOE Lattice Computing project will provide $9.2 million, most of which will be used to expand the clusters.

“For many years the Holy Grail was one dollar per megaflap,” says Holmgren. “In 2000, our cluster was operating at a cost of about 15 dollars per megaflap. This year, we are about there.”

Progress in software

Having enough computing power is only one ingredient in advancing QCD calculations. To efficiently harvest the enormous amounts of computing power now available to the lattice QCD community, scientists also need to optimize the software and the scientific algorithms used in their QCD calculations.

“One tends to emphasize the hardware,” says Sugar. “But the software is really important for these difficult-to-handle machines. The code has to be adapted to the machines.”

Ideally, a lattice QCD application should be able to run both on a cluster system and a QCDOC machine. To achieve this goal, the DOE SciDAC program has provided funding for software development since 2001. The lattice QCD community has designed and implemented a standard QCD Applications Program Interface that provides a uniform programming environment on a variety of computer systems, from PC clusters to supercomputers.

The interface has allowed theorists to focus on optimizing their scientific algorithms and methods. With more computing power now available, they have done away with their crudest approximations and have begun to produce attention-grabbing results.

“With today’s theoretical methods, we still need more computing power,” Sugar says. “The two things go hand in hand. That’s always going to be the case.”
Artist Robert Lang has folded intricate paper sculptures from flat sheets that, in some cases, started out over nine feet long. He uses the same method many of us used to make cranes and party hats in elementary school—a series of precise folds. But Lang’s designs are far more complex. Using advanced mathematics, Lang can fold a snake with 1000 scales from a single sheet of uncut paper. And that’s just the beginning.

Lang is a retired physicist and engineer with a PhD from Caltech. Now a full-time origamist, he creates seemingly impossible designs by breaking complicated geometry problems into a series of steps, or algorithms, that can be solved by a computer. Lang’s algorithms have pioneered a new field of mathematics called “computational origami.”

Lang’s computational origami inspired a young MIT computer science professor, Erik Demaine, to solve a famous geometry problem called “fold-and-cut.” The question is simple: How many two-dimensional shapes can you get by folding a paper any number of times, as if to make a paper-snowflake, and then making only one straight cut? The fold-and-cut problem had puzzled mathematicians for years. But in 1998, after two years of crunching origami algorithms and mathematical proofs, Demaine came up with a surprising solution: you can theoretically create any design—from a snowflake, to a detailed silhouette of the Eiffel Tower—after making just one cut in the paper. “Of course, some shapes are just not feasible in real life,” explains Demaine, “but in theory, literally any shape could be made after just one straight cut.”

Origami has been used to solve engineering problems too. Lang’s algorithms have improved airbags and expandable space telescopes by increasing the area that can fold out from a small...
volume, like a multifaceted pop-up book. Taking these principles even further, bioengineers are now using computational origami to understand how the body works and improve medical devices. Lang’s method could help researchers understand how proteins fold in our bodies, for example, so we can treat protein-folding disorders such as mad cow disease. Origami may also help unclog our arteries by improving the traditional stents used in coronary surgery. A physician can route a tiny origami stent through a blood vessel and then expand it, lodging the device in the larger artery that needs support.

Of course, not all of Lang’s designs save lives; some just look cool. Each piece shown here, from the scorpion with pincers to the winged cicada, was folded from a single sheet of paper. They are vivid, almost eerie, reminders that math can be beautiful.
Scientists at the Laser Interferometer Gravitational-Wave Observatory (LIGO) are hoping to catch a wave—a gravitational one. With computer-coupled observatories in Richland, Washington, and Livingston, Louisiana, LIGO has been analyzing data since 2002 in an effort to detect and measure cosmic gravitational waves. LIGO’s L-shaped detectors uses laser beams and mirrors in hopes of detecting changes in distance between its test masses as small as one-hundred-millionth of the diameter of a hydrogen atom. That change

**DATAFIND**: Data from each of LIGO’s three detectors, H1 and H2 from Washington, and L1 from Louisiana, are distributed across six LIGO computing centers. “Datafind jobs” query catalogs to locate needed data. The depicted inspiral workflow is performed on every 2048-second parcel (about 34 minutes) of data.

**TMPLTBANK**: Using parameters such as mass and spin, and accounting for detector sensitivity, theoretical models are used to make a bank of expected waveforms, or templates, for binary inspiral events.

**INSPIRAL**: Data recorded by LIGO are compared with the waveforms in the template bank and those that match within some statistical threshold are stored for further analysis.

**SINCA + THINCA**: Programs look for coincident events, observed at the same time and with the same mass parameters in two or more detectors.

**TRIGBANK**: The events that survive in coincidence from the Thinca program are converted back into template waveforms.
would indicate a wave’s presence.

The LIGO experiments use grid-computing technologies to handle the collection and analysis of data. This workflow analyzes data looking for inspiral signals, which can occur when two compact objects, such as neutron stars or black holes, form binary systems. Over time, the objects spiral in toward one another, producing gravitational radiation. This diagram illustrates the steps required to turn the raw data collected from those signals into interpretable observations.

> **INSVPETO:** Additional tests are performed to verify that the data matches a template waveform. These tests are computationally costly, so they are only performed on candidate events observed in at least two detectors.

> **THINCA2:** The coincidence step is repeated to find a final list of candidate events. The result of the series of programs is an upper limit on the expected rate of binary inspiral events within the surveyed portion of the galaxy. Once the statistics are calculated using the workflow, LIGO scientists begin to interpret the results. LIGO has performed four science runs since 2002 with the fifth scheduled for late 2005, during which the LIGO instruments will operate at design sensitivity and will collect one year of observational data.

Text: Kendra Snyder
Source: LIGO Collaboration
Bringing the Internet to China

When I was at high school in England my favorite subject was geography/geology. However, fearing that jobs in geology might involve looking for oil in inhospitable places, with few encounters with the opposite sex, I switched to physics. Since then, I earned a PhD in nuclear physics, switched to high-energy physics, and then to computing and networking. More recently, working on monitoring Internet performance at sites in over 120 countries around the world in an effort to quantify the “digital divide”, it appears whatever skills I had in geography have not gone to waste.

My first real exposure to developing countries was in early 1991 when I was invited to attend a meeting at Stanford Linear Accelerator Center with Chinese physicists to discuss the possibilities for computing and networking at the Institute of High Energy Physics (IHEP) in Beijing. Never having been to China, but with a conference trip to Tokyo looming, I wangled an invitation to try to set up a network connection from IHEP to SLAC. Somewhat at a loss to know exactly what I might expect in China two years after Tiananmen Square, and whether or how to proceed, I met with Pief Panofsky, director emeritus of SLAC. He was very encouraging, pointing out the important benefits that good networking could make to HEP and the collaboration between China and the United States.

At that time, IHEP had one fax line that could make international calls, plus a dial-up X.25 phone line to CERN in Europe that was mainly used for transferring mail twice daily. The very least I could do was to request that IHEP install three international phone lines in their computer center. Fearing bureaucracy would impede this, Panofsky enlisted Nobel Prize winner T.D. Lee to help get the phones and quickly obtain a visa for my visit.

On arriving at IHEP three weeks later, I met with the IHEP computing staff. They were excited about working with western “experts” and were determined not to let any lack of knowledge of English impede things. I was flattered by their attention, friendliness, and enthusiasm; challenged to make myself understood; and amazed and elated to find the phone lines had been installed the day before. I had brought with me, just in case, two modems, so I quickly attached one to the phone line and the VAX 785 computer. We used the second phone line to call Charley Granieri and others at SLAC to set things up and successfully call the SLAC modem pool. Over the next two weeks, after further experimenting, we set up a DECnet dial-up connection between SLAC and IHEP with an effective transfer rate of 400 bits per second and a cost of about $3 per minute.

After returning to the United States, we quickly convinced Bob Woods at the Department of Energy to fund an AT&T satellite circuit between IHEP and SLAC. However, from there on things started to get harder. It took over a year to get links from the satellite station at Beijing airport to IHEP. We tried numerous solutions including infrared and microwave transmission and eventually settled on optical fiber and copper. The satellite link was finished in March 1993 and was a big improvement, providing file copy rates of about 42,000 bits/s and transferring about 2500 email items per day. Word about the link quickly spread in Chinese academic circles; institutions started to connect to IHEP; and over 300 top academicians from all over China got accounts at IHEP so they could email the rest of the world.

By this time it was obvious to us that the next step was to replace the DECnet access with full Internet connectivity. To do this required shipping to IHEP routers that required US Department of Commerce export licenses. After substantial paperwork and communications with the US Departments of Energy, Commerce, and Defense, the license was granted, the routers were received in Beijing in February 1994, and the link opened up to the worldwide HEPnet in March 1994.

The final step of connecting the link to the Internet was achieved on May 17, 1994, following required notification to all ESnet (Energy Sciences Network) sites that the Internet would be carrying Chinese network traffic. This was the first Internet connection to mainland China. The HEP community should be proud to have pioneered the connection: There are now about 100 million Internet users in China.

Les Cottrell

Les Cottrell is the assistant director of computing services at SLAC.
In March 1989 Tim Berners-Lee, a young computer scientist at the European particle physics laboratory CERN sent a memo to his boss, Mike Sendall, with the title “Information Management: A Proposal”. On the cover was a bewildering array of bubbles and boxes with arrows pointing between them. Inside was the blueprint for the World Wide Web. Mike had a reputation for recognising a good idea when he saw one. “Vague,” he wrote on the cover, “but exciting.”

and he encouraged his young protégé to continue. The following year, Berners-Lee set to work on the first browser and server, defining the concepts of HTTP, HTML, and the URL. By Christmas, the Web was up and running...between two offices at CERN.

In 1994, CERN put the Web software in the public domain, ensuring that it would remain an open standard. Today, the Web has by far outgrown its origins, but it is no accident that it began as a collaborative tool for particle physics. **James Gillies, CERN**
The Grid

Having bought a new toaster, we simply plug it in: the electric power grid removes the need to also buy and install a new generator. By analogy, information technologists refer to “the Grid” when talking about on-demand computing.

Like its electrical namesake, a computing grid is a mix of technology, infrastructure, and standards. The technology is software that allows resource providers (whether individuals or institutions) to contribute computers, storage, data, networks, and other resources; it allows consumers to use them when needed. The infrastructure comprises the physical hardware and services that must be maintained and operated for the resource-sharing to occur. Finally, standards codify the messages that must be exchanged, and the policies that must be followed, to allow a grid to function.

The Internet, Web, and Grid are related but distinct technologies. The Internet is the worldwide system of networks that connects many computers and smaller networks, allowing them all to communicate. The Web is a way of accessing information over the Internet. The Grid is a way of using the Internet to share and manage computing resources that are distributed around the globe.

Ian Foster, Argonne National Laboratory and the University of Chicago