The TeraGrid mission is to enable and support world-class computational research and to promote science and technology education through the provision of an advanced, distributed, comprehensive, and open cyberinfrastructure.

TeraGrid Resource Providers:

- Indiana University (IU)
- Louisiana Optical Network Initiative (LONI)
- National Center for Atmospheric Research (NCAR)
- National Center for Supercomputing Applications (NCSA)
- National Institute for Computational Sciences (NICS)
- Oak Ridge National Laboratory (ORNL)
- Pittsburgh Supercomputing Center (PSC)
- Purdue University (Purdue)
- San Diego Supercomputer Center (SDSC)
- Texas Advanced Computing Center (TACC)
- University of Chicago/Argonne National Laboratory (UChicago/Argonne)
<table>
<thead>
<tr>
<th>Page</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>Teragrid Leadership</td>
</tr>
<tr>
<td>3</td>
<td>XD: The Future is Now</td>
</tr>
<tr>
<td>4</td>
<td>When Hearts Go Wild</td>
</tr>
<tr>
<td>6</td>
<td>Finding a Leader in a Crowd</td>
</tr>
<tr>
<td>8</td>
<td>In Sequence</td>
</tr>
<tr>
<td>10</td>
<td>How Spiders Spin Silks of Superhero Strength</td>
</tr>
<tr>
<td>12</td>
<td>Solving an Earth-Sized Jigsaw Puzzle</td>
</tr>
<tr>
<td>14</td>
<td>When Cellular Bones Soften</td>
</tr>
<tr>
<td>16</td>
<td>Oil, Oil Everywhere</td>
</tr>
<tr>
<td>20</td>
<td>Counting Comets</td>
</tr>
<tr>
<td>22</td>
<td>The Need for Nanospeed</td>
</tr>
<tr>
<td>24</td>
<td>Decoding Deafness</td>
</tr>
<tr>
<td>26</td>
<td>Supercomputer Sheds Light on HIV’s Behavior</td>
</tr>
<tr>
<td>28</td>
<td>Dawn of the Giants</td>
</tr>
<tr>
<td>30</td>
<td>Cloud Computing—Literally</td>
</tr>
<tr>
<td>32</td>
<td>Asking “What If?” About H1N1</td>
</tr>
<tr>
<td>34</td>
<td>Data Mining New Materials</td>
</tr>
</tbody>
</table>
TeraGrid Leadership

Top Row: Sean Ahern (NICS); Phil Andrews (NICS); Jay Boisseau (TACC); John Cobb (ORNL); Ian Foster (UChicago/Argonne-GIG); Geoffrey Fox (IU); Thomas Furlani (SUNY Buffalo); Kelly Gaither (TACC); Middle Row: Matt Heinzel (UChicago/Argonne); Daniel S. Katz (UChicago/Argonne); Scott Lathrop (UChicago/Argonne); Honggao Liu (LONI/LSU); Michael Levine (PSC); Rich Loft (NCAR); Richard Moore (SDSC); Mike Norman (SDSC); Bottom Row: Mike Papka (UChicago/Argonne); Ralph Roskies (PSC); Barry I. Schneider (NSF); Carol Song (Purdue); Craig Stewart (IU); John Towns (NCSA); Nancy Wilkins-Diehr (SDSC); Jeffrey Vetter (NICS/Georgia Tech).

For more information see TeraGrid leadership at: https://teragrid.org/web/about/senior-management
Mid-2011 will see the launch of the next phase of the National Science Foundation’s (NSF) investment in high-end computing: the eXtreme Digital, or XD, program, which will supplant the TeraGrid program. XD will increase the productivity of the computationally savvy researchers who use our resources, and the new infrastructure will enable major advances in science and engineering.

This isn’t the first time we’ve faced such a transition. Many of us were present when the first high-performance computing centers were launched in 1986. We were there in 1997 when NSF created significantly larger partnerships of institutions with a range of computing systems and a distributed staff of more than 200 experts. This program, Partnerships for Advanced Computational Infrastructure, consolidated the allocation of storage, computational time, and advanced user support. This concept further evolved with the birth of TeraGrid, the current generation of NSF-funded cyberinfrastructure (CI). Today there are nearly 400 members of the TeraGrid team who manage and support 24 diverse systems representing nearly two petaflops of computational power, hundreds of software applications, more than 100 databases, and 50 petabytes of storage at 11 sites across the continental U.S.

Most TeraGrid resource providers are involved with one of the two competing bids for the management of the XD project. Regardless of which team is selected to manage the next phase change in this 25-year history, they will capitalize on their in-depth knowledge and NSF’s sustained commitment.

As we await the results of the XD competition, we can rest assured that TeraGrid “lessons learned” will shape the future. The NSF’s vision for XD began in 2007 when they published their strategic plan for a “national-level, integrated system of hardware, software, data resources, and services…to enable new paradigms of science.” In 2010, the “Cyberinfrastructure Framework for 21st Century Science and Engineering (CF21)” document described a culture that focuses on the integration of resources, and not the resources themselves. In addition to meeting the CI needs of U.S. researchers who aim to solve scientific grand challenges, it recognized the importance of integration with other academic, regional, commercial, agency, industry, and even global counterparts. In 2009, six task forces, with representatives from dozens of national institutions, and led by members of the NSF Advisory Committee for Cyberinfrastructure (ACCI), began a 12- to 18-month effort to develop recommendations for improvements. These reports should be completed in the coming months and will provide guidance in developing the future environment of advanced digital services to enable transformative achievements in science and engineering.

Hardware investments will also shape the future. Some current TeraGrid systems will continue into XD, and new ones will be added, as has been the case during the last 25 years. Through the initial XD awards, the Technology Audit Service and Technology Insertion Service, which began in 2010, XD will have systemic tools in place to benchmark user satisfaction and resource utilization across the board. It will also have a means by which to identify the most promising technologies to meet evolving demands. These measures will allow us to be better stewards of XD resources and optimize their use by an increasing number of users and new fields of research that we are committed to continue to engage.

We are in the business of driving scientific discovery by ensuring researchers’ access to the computers, resources, and expertise they need. The hardware may change, the name of the program may change, and some of the faces may change. Collectively, our commitment hasn’t changed in 25 years, and it won’t change with the XD program.

As chair of the TeraGrid Forum, it’s my pleasure to share this collection of science and engineering highlights. They reflect that commitment. But, more importantly, they represent some of the best work of our TeraGrid users and the breakthroughs they are making a reality. Enjoy reading about the scientific advances TeraGrid made possible in 2010, and imagine what the future will hold!
A novel, low-energy defibrillation method shows promise to reduce pain and tissue damage for millions who suffer heart arrhythmias.
Like a big kick in the chest—that’s how people who have undergone defibrillation while conscious often describe it. Applied externally with “paddles” or by implantable devices, defibrillation applies a brief burst of electrical current at energy levels many times higher than the human pain threshold.

“It’s a huge shock, 130 to 360 joules externally, about seven internally,” says computational scientist Elizabeth Cherry of the Rochester Institute of Technology (RIT, formerly at Cornell). “Basically, conventional defibrillation is for emergencies, most often ventricular fibrillation (VF), which is almost always life-threatening and requires immediate resuscitation,” says Cherry, whose work focuses on the heart’s complex electrophysiology.

Many other cardiac arrhythmias, however, especially atrial fibrillation (AF)—affecting about 2.2 million Americans—may present serious health problems that can be treated with defibrillation—if it didn’t involve serious pain and risk of lasting tissue damage.

“The idea of Far-Field Antifibrillation Pacing, or FFAP,” explains Cherry, “is that you apply a pulsed electric field, and as it encounters discontinuities, such as blood vessels, collagen and other things, it recruits these discontinuities as virtual electrodes. In this way, many new activations develop simultaneously throughout the heart, which synchronize electrical activity and restores normal rhythm.”

Toward that end, in studies involving both laboratory experiments and computational simulation, Cherry and a large group of collaborators, including physicists Flavio Fenton (Cornell), Jean Bragard (University of Navarra, Spain), and others at Cornell and the Max Planck Institute (Göttingen, Germany), conducted a research program that combines clinical, experimental, and theoretical perspectives with computer simulation. Because of the great range of scales involved in heart anatomy—both spatially (from a single cell to the full-size heart) and over time (microseconds to minutes)—their modeling requires large amounts of computing. For their whole-organ model of cardiac electrical dynamics, they relied on PSC’s BigBen (up to 500 processors simultaneously) until it was decommissioned this year, and are now moving their code to Purdue’s Steele system, both TeraGrid resources.

The FFAP studies focused on AF, an arrhythmia in the heart’s upper chambers. AF often arises with age and, unlike VF, can persist for years. Although AF seldom requires emergency treatment, it increases risk for stroke and heart failure. Current treatments, primarily anti-arrhythmic drugs and sedated defibrillation in a clinical setting (called cardioversion), aren’t especially effective and often have side effects. “There’s a big clinical hole,” says Cherry, “in how to treat this type of disease.”

Their heart experiments with FFAP have shown a success rate comparable to conventional defibrillation, higher than 90 percent, in stopping AF and restoring a normal heartbeat. Their computational simulations correlated with these experiments confirm the theory underlying FFAP and make it possible to test many possible remedies. Cherry and her team reported their findings last year in Circulation (August 2009), and newer publications are in press.

“Based on pain threshold values in the literature,” says Cherry, “we believe our approach is currently at the threshold and that with optimization of parameters such as shock waveform and electrode placement, guided by computer simulation, we’ll be below it.”

For more information:
http://thevirtualheart.org/FentonCherry/cherry.html
Grant #s: NSF 0800793, BES-0503336
Finding a Leader in a Crowd

Wikipedia study is a model for understanding Internet-driven collaborations

This visualization shows relationships between users—so-called “betweenness centrality”—who worked on a sample of the Wikipedia articles created between 2001 and 2008, all of which are being examined in a Purdue study. Courtesy: David Braun, Purdue University
From an organizational perspective, Wikipedia and other collaborative network-driven projects may be less like a new, egalitarian way of doing things and more like an old-fashioned factory floor.

In theory, Wikipedia’s entries are created, edited, and maintained with little in the way of traditional, hierarchical organizational and leadership structures. Its production has been likened to an ant colony, resulting from the collective actions of individual participants with the “wisdom of the crowd” yielding a viable result.

To test this view, Purdue researchers led by Sorin Adam Matei are analyzing the entire collection of articles produced in Wikipedia from 2001-2008, and all their revisions—a computationally demanding task made possible by TeraGrid resources.

“We looked at how article production is distributed across users and users’ contributions relative to each other over time. The work includes visualizations of patterns to make them easier to discern,” says Matei.

Early results, highlighted at the 2009 international Wikimania conference, suggest that Wikipedia isn’t as communal, egalitarian, and free of division of labor as previously thought. Hierarchies featuring bosses and workers, elites and the not-so-elite, have developed. This may, in fact, be necessary when humans organize to produce something as complex as an encyclopedia, despite the essentially democratic nature of network technologies that can, theoretically, allow anyone to participate equally.

“We need to reconsider the way we think about these environments,” says Matei, a Purdue communications professor. “There’s a tendency for the collaboration to become centralized, to become dominated by specific voices, which leads to much more structure than we would imagine.”

David Braun, a research computing specialist working with Matei, says their analysis, for example, has identified Wikipedia users responsible for hundreds of articles.

“The distribution of effort has increasingly become more uneven, unequal,” Matei says.

Braun, a member of Purdue’s TeraGrid staff, says TeraGrid computational resources make processing the voluminous Wikipedia text feasible. Intensive calculations examine participation by millions of people and generate a measure of “entropy,” in other words how structured or unstructured the process is, at numerous points over articles’ lifetimes.

Purdue is creating an online repository of Wikipedia data and an analysis tool available to any researcher. Matei already has developed a small application, called Visible Effort, for calculating entropy on websites using MediaWiki, the software behind Wikipedia and many other wiki sites.

For more information: http://matei.org/ithink/2009/09/18/structure-of-collaboration-on-wikipedia/
http://matei.org/ithink/ambiguity-conflict-wikipedia/
Grant #: TG-CDA090004
In Sequence

TeraGrid systems help University of Illinois physicists imagine next-generation gene sequencing techniques.

Researchers visualize DNA transport through synthetic nanopores. The figure shows an atomic-scale model of a nanopore (gray surface), DNA (yellow and purple strands), and Cl– and K+ ions (red and blue spheres). Water molecules are not shown. Courtesy: Aleksei Aksimentiev, University of Illinois at Urbana-Champaign
The first human genome took 13 years and $3 billion to produce. Today, geneticists can generate the same information in a matter of months for a fraction of the cost.

As next-generation gene sequencers begin to make their mark on the life sciences, teams around the world are racing to develop new and improved DNA sequencers that can ingest a strand of nucleotide bases and directly read a person’s genetic code for less than $1,000.

Aleksei Aksimentiev, a computational physicist at the University of Illinois at Urbana-Champaign, and his team are working to develop a new kind of sequencer that could make the dream of the $1,000 genome a reality.

The sequencer uses an electric field to drive a strand of DNA through a small hole, or “nanopore,” in a membrane. If this process can be controlled, the sequencer will be able to read base pairs in order by measuring the change in current as each pair moves through the hole in the membrane.

A great concept—but does it work?

Not yet, according to Aksimentiev. The experimental designs of these sequencers are plagued by noisy signals, blockages and DNA base pairs that pass too quickly through the pore.

Since experiments can’t show exactly what’s going on inside a nanopore, Aksimentiev produces atom-by-atom models of nanopore designs and sets them in motion using the Ranger supercomputer at TACC (Texas Advanced Computing Center) and the Abe supercomputer at NCSA (National Center for Supercomputing Applications), both TeraGrid resources.

“This intuitively simple physical picture doesn’t apply in practice,” Aksimentiev said. However, his team’s work is uncovering the more complicated picture and how to exploit it for DNA sequencing. His simulations revealed the atomic-level movements of DNA as it wriggled through a nanopore, leading to insights into how to improve the design of the system.

These simulations used the NAMD molecular dynamics code. NAMD is a product of the University of Illinois’ Theoretical and Computational Biophysics Group. For more than a decade, that team has developed the code in part on TeraGrid systems and with occasional expert assistance from NCSA.

“The simulations explain what processes give rise to the signals we measure,” he said.

Aksimentiev discovered that the key requirement for sequencing DNA directly is to keep the strand in the pore long enough to read out its sequence.

“If the DNA moves too fast, then one cannot read out the signal to distinguish the difference between the base pairs,” he said. “We have to find a way to trap the DNA.”

Indeed, Aksimentiev and colleagues believe they’ve built such a trap.

When DNA comes into contact with an electrical field, it stretches. Applying that field on one side of the membrane forces the strands into a pore smaller than it would usually fit. Turning off the field, on the other hand, causes the DNA to relax and traps the molecule in the hole. By pulsing the field, stretching and relaxing the DNA, the strand moves, base-by-base, through the pore at a speed slow enough to be read clearly.

Supercomputers like Ranger and Abe are required for this kind of research because of the precision needed to differentiate between the four DNA nucleotides, which differ by only a few atoms.

The Aksimentiev team filed for a provisional patent in 2009 for their design of the first nanopore sequencer able to accommodate double-stranded DNA.

This work was supported by grants from NIH’s Revolutionary Genome Sequencing Technologies’ program, and NSF’s ‘Physics Frontier Center’ program.

For more information: http://bionano.physics.illinois.edu
Grant #s: PHY-0822613, DMR-0955959 CAREER
How Spiders Spin Silks of Superhero Strength

TeraGrid resources help reveal structures that could lead to a new class of super strong materials.

The strength of biological material such as spider silk lies in the specific geometric configuration of structural proteins. The Massachusetts Institute of Technology’s (MIT) Civil and Environmental Engineering (CEE) department, in collaboration with SDSC researcher Ross Walker, found that this structure is as strong as steel, even though the “glue” of hydrogen bonds that hold spider silk together at the molecular level is 100 to 1,000 times weaker than steel’s metallic bonds. Courtesy: Markus Buehler, MIT; Ross Walker, San Diego Supercomputer Center, UC San Diego
Spiders first spun onto the scene in the summer of 1962 with his ability to produce super-strength strands from “web shooters” with which to fight his foes. For far longer than that, real spiders and silkworms have eluded scientists’ efforts to discover just what makes these strands stronger than steel on a pound for pound basis.

Now researchers at the Massachusetts Institute of Technology’s Center for Materials Science and Engineering, with help from the San Diego Supercomputer Center (SDSC) at UC San Diego and the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign—all TeraGrid partners—have unraveled part of this mystery using detailed supercomputer simulations to better understand the specific geometric configuration within the structural proteins of spider silk.

The team developed the first complete atomistic model of spider dragline silk, which had remained elusive until now. Researchers were able to predict the configurations of silk protein assemblies at the nanoscale, and probe their mechanical properties, i.e. flexibility, extensibility, and strength. SDSC researcher Ross Walker provided support by optimizing the code for the simulations, and assisted with large-scale data transfers to and from the supercomputers used.

The key to the silk’s strength, say researchers, is its beta-sheet crystals, or the nano-sized cross-linking domains holding the material together. Using those supercomputer simulations, Markus Buehler, the Esther and Harold E. Edgerton Associate Professor in MIT’s Department of Civil and Environmental Engineering and Principal Investigator of the Laboratory for Atomistic and Molecular Mechanics, and his team were able to determine exactly how the components of these beta sheet crystals interact with each other.

They found that an unusual arrangement of hydrogen bonds, or the “glue” that stabilizes the beta-sheet crystals, plays an important role in defining the strength of silk. These hydrogen bonds, which are among the weakest types of chemical bonds, gain strength when confined to spaces on the order of a few nanometers in size. Once in close proximity, the hydrogen bonds work together and become extremely strong.

“Tiny crystals in silk are stronger, and have the ability to quickly re-form their broken bonds,” explains MIT doctoral graduate Sinan Keten, who assisted Buehler. “As a result, silk fails ‘gracefully’—that is, gradually rather than suddenly.”

This geometric make-up gives spider dragline silk outstanding physical properties. Spider silk’s tensile strength, or how far it can be stretched before it breaks, is superior to that of high-grade steel; in fact, it can stretch up to 140 percent of its length. It is also lightweight: if a single strand was stretched around the earth’s circumference, it would weigh less than one pound.

“We found that the structure of spider silk at the nanoscale can explain why this material is as strong as steel, even though the ‘glue’ of the hydrogen bonds holding spider silk together at the molecular level is 100 to 1,000 times weaker than steel’s metallic bonds,” says Buehler.

The research has implications beyond just understanding the properties of spider silk, says Buehler. “These findings could be applied to a broader class of biological materials, such as wood or plant fibers, or bio-inspired materials such as novel fibers, yarns, and fabrics, or even tissue replacement materials, to produce a variety of useful materials out of simple, commonplace elements.” The longer-term impact of this research could be the development of a new material design paradigm leading to the creation of strong, lightweight and extremely durable materials out of abundant, inexpensive resources.

However, nature has its limits, just like the fictional Spider-Man. One surprising result from the research is that there appears to be a failure point directly related to the properties of spider silk on the exact size of these beta-sheet crystals within the fibers. When the crystal size is about three nanometers—literally only billionths of a meter—the material exhibits its optimum tensile and ductile strength. Anything more than five nanometers, however, and the material will lose strength and become brittle.

But for both superheroes and scientists, this may only make for an even better sequel.

For more information: http://www.nature.com/nmat/journal/v9/n4/abs/nmat2704.html
http://rsif.royalsocietypublishing.org/content early/2010/06/01/rsif.2010.0149.abstract
Grant #s: TG: TG-MSS080030; NSF: CMMI-0642545, MRSEC DMR-0819762
TeraGrid simulations map the movement of the Earth’s mantle.

Solving an Earth-Sized Jigsaw Puzzle

Tectonic plate motion (arrows) and viscosity arising from global mantle flow simulation. Plate boundaries, which can be seen as narrow red lines, above insert are resolved using an adaptively refined mesh with 1km local resolution. Shown are the Pacific and the Australian tectonic plates and the New Hebrides and Tonga microplates. Courtesy: Georg Stadler, Institute for Computational Engineering & Sciences, The University of Texas at Austin.
long parts of the sea floor, jostling junctions in the earth’s crust known as tectonic plates can move extremely fast. Nowhere is this more evident than in the southwest Pacific, where plates fall into the mantle in a process called trench rollback and cause two plates to converge at a rate of 25 centimeters per year, nearly 10 times faster than the speed of tectonic plates elsewhere.

“It’s one of the most spectacular phenomena to happen within the planet’s interior,” according to Michael Gurnis, professor of geophysics at the California Institute of Technology (Caltech) and Director of the Seismological Laboratory.

The standard model of plate tectonics is many decades old, but researchers have never been able to simulate the complex dynamics of the mantle with sufficient detail to explore the massive geological divides in the earth’s surface where earthquakes and volcanic eruptions occur, and where microplates race toward one another.

“This phenomenon has eluded numerical simulation for years,” explains Gurnis. “When it emerged in our simulations of the whole planet, to be honest, it was a surprise.”

In 2007, researchers from Caltech and The University of Texas at Austin were awarded a Petascale Applications (PetaApps) grant from the National Science Foundation (NSF) to use computer modeling to answer some of the most pressing questions in geophysics: What controls the speed of plates? How do microplates interact? How much energy do the plates generate and how much energy do they dissipate?

“NSF created this program to challenge groups to gear up for the petascale era,” says Omar Ghattas, Jackson Chair in Computational Geosciences in the Departments of Geological Sciences and Mechanical Engineering and in the Institute for Computational Engineering and Sciences at The University of Texas at Austin.

In addition to correctly modeling microplates in the southwest Pacific, the research team produced simulations that depicted the subsurface forces at work in the powerful February 2010 earthquake in Chile.

The group’s simulations also overturned a long-held notion in geophysics that the bending of submerged plates dissipates most energy in the Earth.

“We discovered that there is an enormous amount of dissipation where plates bend, but in terms of the total energy release, it’s actually a small factor,” Gurnis explains. “This means there is dissipation throughout almost the whole interior and not just in one place.”

In preparation for the arrival next year of the 10 petaflops NSF Blue Waters system at the National Center for Supercomputing Applications (NCSA), the team has scaled their code to over 100,000 processors on Jaguar at the Oak Ridge National Laboratory (ORNL), with the multiresolution algorithms scaling to over 200,000 cores — the absolute limit of today’s technology.

“It’s almost as if we jumped over a whole generation of computation in the sense of being able to reproduce the fine-scale details of deformation near earthquakes in a global model,” Gurnis says.

For more information: http://www.sciencemag.org/cgi/content/full/329/5995/1033

Grant #s: NSF’s PetaApps program (OCI-0749334, OCI-0748898)
Biomolecular simulations reveal fundamental knowledge that could help the search for new anti-cancer drugs.
Actin, so named because it activates muscle cells, is the most abundant protein by mass in the body. Basically, where there’s life there’s actin. In evolutionary terms, it’s highly conserved, meaning it’s present to some degree in the most simple to complex species of “eukaryotic” organisms—any living thing made of cells with a nucleus.

Perhaps foremost among actin’s important functions is structural engineering. As bones are to the body, actin is to cells. Just beneath the cellular membrane, actin forms networks of filaments that are a primary component of the cytoskeleton, an undergirding molecular structure that maintains cellular shape, protects the cell and—with its ability to dynamically extend and contract—enables cellular motion.

“One of the most important things in cell biology is the behavior of the cytoskeleton and what proteins do to drive this behavior,” says Greg Voth, a chemist at the University of Chicago. “We’ve learned a lot over the years about actin, how it forms polymers and then changes its flexibility properties and depolymerizes. This cycle is what cells use to create motion, change shape and to do many other things, and it’s at the core of cellular behavior.”

The fundamental processes by which individual actins link with each other (polymerize) to form filaments and, in turn, break apart (depolymerize) have been found to be involved in various cancers, in particular breast cancer. “There’s a lot of interest in cancer that goes along with this kind of fundamental cellular biology,” says Voth. “People would like to find drugs that target cancer cells, but you can’t design drugs of this kind until you understand these fundamental steps.”

Gregory Voth, University of Chicago
Jim Pfaendtner, University of Washington
Jim Pfaendtner of the University of Washington uncovered previously unknown details of these fundamental processes.

They first looked at how one small part of actin’s structure changes during metabolism, a question raised by laboratory experiments. For this work, they used molecular dynamics software called NAMD with the Ranger system at TACC, where PSC scientist Phil Blood, working through the TeraGrid ASTA program optimized NAMD to run 30 percent faster than was previously possible, using up to 2,000 processors simultaneously.

They went on to simulate multiple actins combined into filaments and how they interact with other biomolecules. They collaborated closely with experimentalists to corroborate their findings. “TeraGrid has enabled this experiment-based collaboration,” says Pfaendtner, “and through it we’ve seen the experimental community becoming enthusiastic about what we can do with simulations.”

Their results—reported in Proceedings of the National Academies of Sciences and The Journal of Molecular Biology—show that these interactions make actin filaments structurally more flexible, in effect softer, initiating the structural change that leads to the breaking apart of the filaments. “We’ve been really surprised,” says Voth, “to find how relatively small changes at the molecular scale propagate to properties of the cytoskeleton. This is very fundamental knowledge that we’re getting from these simulations.”

For more information: http://www.cheme.washington.edu/people/faculty/pfaendtner.htm
Grant #: NSF OISE-0700080
Researchers use TeraGrid’s advanced computing and networking to aid Gulf of Mexico oil spill response.
When the blowout of the British Petroleum (BP) Macondo well destroyed the Deepwater Horizon oil rig in the Gulf of Mexico on April 20, 2010, it touched off the largest environmental disaster in U.S. history, leading to a full-scale effort to stop the leak, assess the full scope of the damage, and take steps to minimize further harm.

At universities across the nation, researchers used advanced cyberinfrastructure available through the Texas Advanced Computing Center (TACC) and Louisiana Optical Network Initiative (LONI), both TeraGrid resource providers, to help inform the response effort and forecast the oil spill’s impact throughout the Gulf Coast region.

Gordon Wells, a researcher at The University of Texas at Austin’s Center for Space Research (CSR), was the first person to see satellite images of the BP disaster on a daily basis. Wells’ group was monitoring conditions in the south-central U.S when the explosion occurred. He immediately began to relay CSR’s direct broadcast satellite imagery of the area to the National Oceanic and Atmospheric Administration’s (NOAA) marine pollution surveillance team, which organized the monitoring effort.

With the assistance of data management experts at TACC, Wells streamed this data—several terabytes a day—to about 30 national and local relief agencies and thousands of individuals through the TeraGrid-supported high-speed network, as containment and clean-up efforts began.

“The Coast Guard used our information daily to decide where they were going to have an operation, and where they were most likely to intersect with the oil spill,” Wells explains.

This image depicts the movement of oil in the Gulf of Mexico. Satellite images were used to initialize the oil position for the simulation. The lines represent the hypothetical path of oil based on weather forecasts. The data was visualized by TACC staff using the Longhorn visualization cluster. Courtesy: Univ. North Carolina at Chapel Hill, Institute of Marine Sciences; Univ. Notre Dame, Computational Hydraulics Laboratory; Univ. Texas, Computational Hydraulics Group, ICES; Univ. Texas, Center for Space Research; Univ. Texas, Texas Advanced Computing Center; Seahorse Coastal Consulting
High-Speed Connections Aid Response Teams

Also responding immediately to the oil spill was LONI, a high-speed, fiber optic network that connects supercomputing resources among six universities and two Louisiana State University (LSU) health sciences centers.

LONI provided the NOAA team with access to its high-speed, high-bandwidth networking connections so they could share and transfer critical data quickly from New Orleans. Because there is no central NOAA office in Louisiana, the response teams would otherwise have been forced to use commodity Internet connections to transfer large amounts of data to NOAA’s Washington, DC headquarters.

“Through LONI, we were able to assist the NOAA staff so they could send updates in a timely manner and work more effectively than if they had to rely on a traditional network,” said Donald Vandal, LONI Executive Director.

Another Louisiana group aiding in the early stages of the Gulf Coast clean-up was CLEAR, (Coastal Louisiana Ecosystem Assessment and Restoration), a collaboration among federal, state, and university researchers that analyzed various data sets to advise on coastal recovery and restoration efforts. Assisting in this process was PetaShare, a distributed data management system that Tevfik Kosar, a professor with LSU’s Department of Computer Science, created through a grant from the National Science Foundation (NSF). Kosar provided the CLEAR team with access to PetaShare to aid them in the data analysis. Using PetaShare allowed multiple researchers to analyze data from one central location, thereby reducing their research time.

Predicting the Spill’s Spread

If providing satellite imagery and access to data was the first step in understanding the immensity of the spill and tracking its progress, the next step was using this information to predict the movement of the spill, and to forecast the potential impact of a hurricane in the region.

Clint Dawson, head of the Computational Hydraulics Group at The University of Texas at Austin’s Institute for Computational Engineering and Sciences (ICES) and a colleague of Wells, marshaled TeraGrid resources by receiving an emergency three-million-hour allocation from the NSF to apply computation modeling and prediction to the oil spill.

Working with Rick Luefttich (University of North Carolina Chapel Hill) and Joannes Westerink (University of Notre Dame), Dawson and his group used ADCIRC (Advance Circulation Model for Coastal Ocean Hydrodynamics), the leading storm surge model, to predict how the massive spill might affect hundreds of miles of coastline in the region.

Dawson, an authority on the specific dynamics of the Gulf’s tides, currents, and wave systems, used the Ranger supercomputer at TACC to create daily forecasts of the oil spill’s movements based on ADCIRC model, showing how it might migrate over a 72-hour period. The high-resolution models forecast the spill spreading toward Texas days before any tarballs washed ashore on the upper Texas coast. These forecasts helped first responders position
booms along the shore, directed U.S. Coast Guard ships to the thickest plumes of oil, and helped prepare emergency teams for the possibility of a natural disaster—a hurricane—compounding one of the nation’s worst man-made disasters.

In late June, with Hurricane Alex approaching the Gulf Coast region, Dawson’s team simulated the storm surge based on advisories issued by the National Hurricane Center. Within two hours, researchers produced forecasts, processed the results, and sent them to Wells at the Texas State Operations Center.

Those simulations provided 50-meter resolution for the near-shore regions of interest—10 to 20 times more detailed than other models of the oil—and were used to provide a 72-hour forecast, letting state offices position emergency personnel appropriately to protect coastal areas in the event of a hurricane.

“Having the storm surge model allowed us to isolate areas in danger, and to get search and rescue teams out there to do operations and do them effectively,” says Wells.

Adding Oil to the Storm

Most hurricane and storm surge forecasting models are not designed to consider the three-dimensional movement of a large oil spill. For more effective predictions and response, scientists needed to combine models using different physics and examine multiple elements simultaneously.

A team of LSU researchers performed complementary storm surge research using LONI’s resources. Q. Jim Chen, with the Department of Civil and Environmental Engineering, and Robert Twilley, with the LSU Department of Oceanography, created a hurricane and storm-surge forecasting model that incorporated deposit and movement of oil into their predictions. Because these complex models involve massive data sets, Chen’s and Twilley’s teams used LONI to develop and integrate multiphysics models and automate the data input to create visualizations rapidly.

Another LSU professor, Mayank Tyagi, with the Department of Petroleum Engineering, used LONI resources to investigate how spilled oil flows through water. Tyagi’s research in this area focuses mainly on computational fluid dynamics, the study of fluid flows in nature. Tyagi and his team built on their previous models, which were created to explore how oil flows through wells and pipelines, to create new simulations that show how oil from the leak could move through the Gulf and into ocean water. According to Tyagi, these simulations provided a more accurate estimate of flow rate, pressure, and properties of discharged oil at the leak location.

“Situations like these show why advanced networking environments like those available through TeraGrid are valuable to scientific research, especially in situations where response times are critical,” says LONI’s Vandal.

For more information: http://magic.csr.utexas.edu/
http://www.adcirc.org/
http://www.ices.utexas.edu/
Grant #: NSF: 1042318
Counting Comets

Researchers use TeraGrid to shed light on long-term astronomy debate
According to hypothesis, the birthplace and nursery of so-called long-period comets is a spherical cloud about a light year away from the Sun. Here, at the outer-most regions of our solar system, objects largely composed of ices—such as water, ammonia and methane—coalesce and move about in orbits for eons until another force, such as a passing star or gravity of the Milky Way itself, dislodges one, hurling it toward the solar system’s inner sanctum.

Some worry that a celestial intruder such as this may one day collide with Earth, causing a massive geological and biological upheaval. Indeed, scientists believe that an asteroid or series of meteor impacts some 65 million years ago resulted in major climate changes and the extinction of the dinosaurs.

Now, however, researchers Tom Quinn and Nathan Kaib at the University of Washington—using 500,000 CPU hours on the Purdue University cluster Condor—are saying we have little to worry from Oort cloud comets colliding with our planet, settling a long-term issue in astronomy. Essentially, their simulations revealed that the number of comets in the Oort cloud is close to a mere trillion; though seemingly huge, that’s still an order of magnitude fewer than originally theorized. Fewer comets mean milder comet showers and statistically, a reduced chance of one striking the Earth.

Quinn and Kaib used Condor, a software package developed at the University of Wisconsin, which allows computationally complex simulations to be spread across thousands of single processor computers to conduct large N-body simulations of the Sun, the four giant planets (Saturn, Jupiter, Neptune, Uranus), and hundreds of thousands of individual comets. Because each comet has to be tracked for billions of years, in this case 4.5 billion (the age of the solar system), the work required a large number of processors. Quinn said that Condor’s work-sharing architecture made it perfectly suited for this research.

“The formation and evolution of the Oort Cloud requires the calculation of tens to hundreds of thousands of comets over the 4.5 billion-year life time of the solar system. TeraGrid provided us with the necessary 500,000 CPU hours to accomplish this daunting task,” he says.

The Oort cloud is thought to be the home of most long-period comets, or comets with orbits that range from 200 years to millions of years. Hale-Bopp, which awed Earthlings in 1996 and 1997 with its brightness, is thought to belong to the Oort cloud family.

“Evidence for the existence of the Oort cloud can be found from the one or two comets that enter the inner solar system each year,” says Quinn. It was originally theorized that the vast majority of observable long-period comets came from the distant Outer Oort cloud, since these comets were the only ones close enough to passing stars to have their orbits affected by the stars’ gravities.

The results of Kaib and Quinn’s simulations, published July 30, 2010 in Science Express, revealed a dynamic pathway that brings the Inner Oort cloud comets into the solar system on a regular basis. Essentially, they enter the outer solar system due to perturbations from passing stars, after which outer planets—such as Neptune and Uranus—further pull them into orbits that throw them into the inner solar system.

“There’s a bit of badminton going on,” notes Quinn, adding that because the observable comets were thought to only represent the outer region of the cloud, the total number of comets was overestimated by an order of magnitude, a finding that helps us to more accurately represent our galactic neighborhood.

Quinn and Kaib’s research represents one more example of how, with the help of TeraGrid resources, investigators are slowly but surely unraveling the secrets of nature, from the nanoscale to the distant Solar System to the outer reaches of the Universe.

For more information: http://www.astro.washington.edu/users/kaib/work.html
Grant #: NSF:0448721
The Need for Nanospeed

Engineers use TeraGrid systems to explore next-generation transistors and new smart materials.
For nearly two generations, technology has advanced at an exponential pace, with computers increasing their capability by a factor of two every 18 months, as suggested by Moore’s Law. However, this exponential speed-up is now being threatened. The culprit: quantum physics and atomic granularity.

Technology’s rapid growth is based on engineers’ ability to shrink transistors—built generally from silicon—to seemingly impossible small scales. However, when silicon reaches a certain size—10 nanometers, or 5,000 times thinner than a strand of hair—new factors related to the discreteness and quantum behavior of atoms make a considerable impact.

As a consequence, nano-transistors heat to combustion, and particles display exotic traits. Materials we thought we understood need to be evaluated through this new nano-lens, and quantum mechanics must be considered when designing ultra-small systems.

Researchers using TeraGrid systems at the Texas Advanced Computing Center (TACC), the National Institute for Computational Sciences (NICS), and Purdue (Network for Computational Nanotechnology or NCN) are pushing the limits of our knowledge by developing a new generation of nano-transistors and “smart” materials.

Because electrons don’t move quickly through silicon, there are intrinsic limits to the speed at which silicon-based transistors can calculate. Therefore, scientists are searching for alternatives. Mathieu Luisier and Gerhard Klimeck of Purdue University are collaborating with Jesus Del Alamo at the Massachusetts Institute of Technology to explore ultra-small, high-mobility transistors that use a promising alternative to silicon: gallium arsenide, or GaAs.

Gallium arsenide has high electron mobility and is able to convey energy from one electron to another at the nanoscale—good qualities for a transistor. Using the nanoelectronic simulation tool, OMEN, the researchers simulated the quantum behavior of atoms in experimental nano-scale transistors and, for the first time, replicated the observed currents passing through the device.

“We reproduced their experimental data in both the ‘on’ and ‘off’ states of the device, which could only be achieved by properly accounting for the tunneling currents flowing through the insulator layers of the devices,” says Luisier. “OMEN is the only device modeling tool that is capable of such physical accuracy and scaling.”

The simulations used more than 70,000 processors simultaneously, and are helping to determine the optimal size and atomic configuration for this new transistor, which researchers hope will drive computer advances for decades.

“How many atoms thick should you make each of several layers? How long should the channel be to get the best performance?” asks Luisier. “What kind of metal alloy should be used for the transistor gate? These are some of the technology and design challenges where we can help.”

Semiconductors aren’t the only nano-materials worth studying. Thomas Truskett, a chemical engineer at The University of Texas at Austin, is investigating a related, but different question: How do you get molecules to line up faster in new nano-materials?

Truskett is interested in making “smart materials” whose purpose is embedded into their very structure. Examples include gels that harden on impact to become stronger than Kevlar, or metals that “heal” themselves.

Designing smart materials requires an understanding of the processes materials undergo at the smallest scales, and a theory of how to control these processes. Through a series of computational experiments using TACC’s Lonestar supercomputer, Truskett accelerated the movement of virtual particles by grafting a “fuzzy layer” of polymers to the material’s surface.

“If you provide a gentle force, you can break the structure around the particle enough for it to move quickly through the crowd,” says Truskett.

Allowing particles to pass each other faster accelerates the reaction rate of materials, which means the difference between a viable nanoparticle for industry and one that is impractical. Truskett’s theories have been subjected to atomistic simulations and laboratory experiments to test their validity. The findings were published in the Journal of Chemical Physics in September 2009.

For more information: http://www.che.utexas.edu/~truskett/
NSF grant #: 0448721
Decoding Deafness

Harvard researchers tap power of TeraGrid supercomputers to determine how mutation leads to deafness

A close-up view of the linker region between cadherin-23 is shown during a molecular dynamics simulation in which the protein is stretched from both ends. The simulations mimic in vivo conditions in which tip-link cadherins are stretched during sound mechanotransduction at hair cells of the inner ear. Calcium ions (shown as green spheres) were found to be essential for the mechanical stability of the protein (shown in cartoon and sticks). Courtesy: Marcos Sotomayor, HHMI and Neurobiology Department, Harvard Medical School
Little is known about the protein molecules involved in touch and auditory function, but now a team from Harvard University has resolved the atomic-level structure of a protein essential for sound perception. The structure was then simulated using TeraGrid supercomputers to determine how it functions in hearing and deafness.

Sound becomes an electrical signal in hair cells of the inner ear. These sensitive mechanoreceptors are moved by sound, stretching fine filaments called “tip links” to pull open ion channels and generate electrical signals that are sent to the brain. The tip link is made of two molecules, cadherin-23 and protocadherin-15, which are defective in some forms of hereditary deafness.

A team led by Rachelle Gaudet and David P. Corey used X-ray crystallography to determine the molecular structure of cadherin-23’s tip, with and without a mutation causing deafness. Then the team tested cadherin-23’s elasticity using molecular dynamics simulations on TeraGrid systems at the National Center for Supercomputing Applications (NCSA) and the Texas Advanced Computing Center (TACC).

“In order to understand how the protein responds to forces, we put it in the computer and stretched the protein just as would happen in the inner-ear,” says Marcos Sotomayor, a research fellow in Corey’s lab in the Neurobiology Department at the Harvard Medical School.

Using NAMD on the Ranger system at TACC and the Abe cluster at NCSA, the team performed hundreds of simulations that encompassed up to 355,000 atoms. The powerful machines allowed them to test the elasticity of cadherin-23’s tip in multiple near-physiological conditions.

Analysis of more than five terabytes of data generated by the simulations revealed an essential role for calcium ions in the mechanics of cadherin-23. The protein appears to be stiff in the presence of calcium, but weak without calcium. A deafness-causing mutation was found to alter calcium binding to the cadherin-23 protein, thus reducing its mechanical strength and possibly making tip links prone to rupture, thereby impairing sound perception.

“Using the supercomputers, we were able to see where the calcium is bound, how it’s bound to the protein, and how it modulates the elasticity of the protein,” explains Sotomayor. “That’s something that cannot be done with any other technique.

“The outstanding resources and support provided by the TeraGrid were essential to our work,” he adds. The research was published in Neuron in April 2010.

Adapted from a Harvard Medical School article

For more information: http://www.cell.com/neuron/abstract/ S0896-6273(10)00231-X
Grant #: TG: TRAC MCB080015

Left to right: Rachelle Gaudet, Department of Molecular and Cellular Biology, Harvard University; David Corey, Howard Hughes Medical Institute and Department of Neurobiology, Harvard Medical School; Marcos Sotomayor, Howard Hughes Medical Institute and Department of Neurobiology, Harvard Medical School; Wilhelm Weinofen, Department of Molecular and Cellular Biology, Harvard University
Supercomputer Sheds Light on HIV’s Behavior

TeraGrid resources open new research directions to battle this global disease.

Key mutations in specific amino acids in the CA domain change the Gag structure in the immature virion, perhaps altering the HIV-1 maturation pathway. The domains with the highest degree of structure are shown with yellow dots. Courtesy: Gregory A. Voth, University of Chicago.
Despite nearly three decades of research since AIDS and the precursor HIV became a public health crisis, the most successful treatments currently available consist of antiretroviral drug therapies which, at best, merely slow the infection or the disease’s progression.

Now, with the aid of massively parallel supercomputers, along with new multi-scale computational simulation approaches that span time and distance, from the atomic to near macroscopic scales, researchers are hoping to gain new insights into preventing the early stages of HIV-1 infection, thus destroying the virus’ ability to “hijack” other healthy cells.

“To me, this is a fundamental challenge for biomolecular simulation,” says Gary Ayton, an associate research professor in a research team led by Gregory A. Voth, formerly of the University of Utah’s Chemistry Department, and now with the University of Chicago. “To bridge and span all of these scales (of time and distance) such that we can make a meaningful connection with real experiments offers a potentially new approach to treating this disease.”

With funding from the National Institutes of Health (NIH) and in collaboration with the research groups who have been studying AIDS and HIV since the early 1990s, Voth’s team has employed their multi-scale approach on the University of Tennessee and the National Institute for Computational Sciences’ Cray XT5 Kraken supercomputer to examine specific stages the virus goes through as it spreads throughout the body. The goal: to stop the young virus in its tracks during the earliest developmental stages.

A key challenge for the team was to model the Gag polypeptide, a multi-domain protein which plays an important role in the formation of the immature HIV-1 virion. This immature virion later becomes the mature virus particle that infects additional healthy white blood cells. Using multi-scale simulation approaches, Voth’s team discovered that a few select amino acid residues appear to be crucial for the stability of the entire Gag polypeptide structure. Within the larger context of halting HIV-1 infection, if this structure collapses, the immature virion will not develop, and the infection ceases to spread further as the body routinely flushes out older cells in favor of new ones.

Modeling atomic-level behavior can be done using a popular form of computer simulation called Molecular Dynamics (MD). Used for decades, MD codes employ Newton’s Second Law of Motion to model the time evolution of complex biomolecular systems.

For the HIV-1 virion, its size and complexity required a simulation on the scale of 500 million atoms—roughly three orders of magnitude greater than any current MD code can handle. Additionally, the team needed to examine the virus at varying time and length scales to gather meaningful results. Fortunately, Voth’s team had already developed a highly flexible MD code called TANTALUS. Features of TANTALUS that make it attractive to the virion problem are its coupling with all-atom simulations, its ability to use both forms of MD, and then making meaningful connections between the two.

“Using the techniques we’ve developed, we can calculate a good approximation to the interaction between the coarse grain sites, or the actual behavior of atoms within the virion,” Ayton explains. “You then do MD simulations of those particular regions and either validate or don’t validate that particular interaction. It’s a back and forth thing, and at the end what you hopefully get is predictive capability.”

It is precisely this predictive capability that Voth’s team is aiming for.

“That’s another new challenge for the simulation approach,” Ayton says. “You can either use it to test a theory or to mirror an experiment. So we’re trying to look in both directions, using it to test experiments and inspire new ones.”

If Voth’s findings are proven accurate through additional research, their results could have a profound impact on the course of future biological experimentation.

For more information: http://chemistry.uchicago.edu/faculty/person/member/gregory-a-voth.html
Grant #: NSF: CHE-0628257; NIH: P50-GM082545
Dawn of the Giants

TeraGrid simulations study theories about the origin of planets like Jupiter and Saturn

Visualizations of gas density in a gravitationally unstable disk. Researchers are using simulations like these, facilitated by the TeraGrid to study the effects of an already existing planet’s gravity on the surrounding nebula, and its influence on planet formation. Courtesy: Indiana University
To astronomers, they’re known as the “gas giants”—massive planets like Jupiter and Saturn composed largely of non-solid matter such as hydrogen and helium. Though sophisticated telescopes are discovering even larger gaseous behemoths in solar systems beyond ours, their origins are still shrouded in mystery.

Now, however, a team of astronomy researchers from Indiana University and from other institutions—with the help of TeraGrid resources—is starting to uncover clues that may help settle some questions about gas giant formation. The results may have implications not only for our own solar system, but for other critical astronomical questions.

“Gas giants dominate the structure of planetary systems,” says Richard Durisen, an astronomy professor at Indiana University. “Understanding how gas giants form can help astronomers answer even larger questions such as where in the Universe other Earth-like planets are likely to exist. This, in turn, can guide the search for extraterrestrial life.”

In recent years, more than 450 planets—mostly gas giants—have been discovered around other stars in our galaxy. So, astronomers therefore believe gas giants are relatively common throughout the universe. Astronomers also recognize that the intricate process of planet formation begins in a swirling mass of gas and dust surrounding a nascent star, called a protoplanetary disk. Smaller, rockier planets such as our own planet Earth are created when solids in the disk collide with each other, stick together, and progressively grow into a planet-sized body. The same basic process—known as “core accretion”—is thought to occur with so-called ice giants like Neptune, which are built in the colder regions of the disk.

For a while, astronomers thought gas giants had a similar genesis: start with a rocky core, add gas from the disk, and the result is something like Jupiter. But here, the mystery begins—time gets in the way of this theory. In the standard core accretion picture, it would take many millions of years to form a solid core massive enough to attract a gaseous atmosphere from the disk to grow to the final size of a Jupiter or Saturn. But typically, by then, most of the gas in a protoplanetary disk would have disappeared. Gas giants around other stars can be much more massive than Jupiter, and thus making the premise for core accretion even more problematic. So, Durisen and others have been looking into another possibility.

“Nature clearly found a cosmological short-cut to build at least some of the gas giants,” says Durisen. “We, and others, have been studying such a process where the gas in the protoplanetary disk undergoes a self-gravitating instability and clumps together in a short time, providing the seed around which a Jovian planet can develop quickly.”

Recent simulations and animations by former Indiana Ph.D. student Aaron C. Boley, now a Sagan Fellow at the University of Florida, in collaboration with the Indiana team led by Durisen and Thomas Steiman-Cameron suggest that this process—known as gravitational instabilities (GIs)—may indeed resolve the mystery surrounding the formation of the gas giants in at least some planetary systems. The simulations show that for sufficiently extended and massive disks, gas giant planets can form via direct collapse caused by gravitational instabilities on a time scale of thousands rather than millions of years.

The team, which also includes co-investigators Scott Michael, Aaron C. Boley and Kai Cai, has used Pople, the Pittsburgh Supercomputer Center’s (PSC) SGI Altix 4700 shared-memory system as well as NCSA’s Cobalt to produce more than 50 terabytes of simulation data over the past two years. Indiana University’s Data Capacitor wide area file system facilitates data transfer between IU and Pittsburgh allowing the team to access their results quickly, as if they were generated locally on a computer in their home lab. The simulations are then analyzed at IU using the Big Red supercomputer.

Not only are the simulations helping astronomers understand the origins of gas giants, they’re also offering insights into why some massive planetary embryos may migrate toward the center of the protoplanetary disk, while others remain on the periphery.

“Preliminary results from my dissertation studies show that GIs can accelerate the inward migration of newly formed gas giants, but that, in regions where the disk is not susceptible to GIs, the inward migration is slowed or halted altogether,” adds Scott Michael, one of Durisen’s current doctoral students.

“This may explain why planets are not always drawn into the central star. In an inactive laminar disk without GIs, migration is expected to cause gas giants forming by core accretion to drift inward rapidly.”

Grant #s: NASA: NNG05GN11G; NSF: CNS0521433
TeraGrid helps researchers clear the skies for better climate modeling

A snapshot from a global cloud-system-resolving model simulation of May 21-August 31, 2009, showing a sector of Earth including eastern Asia and the western tropical Pacific Ocean, with cloudiness (based on outgoing long-wave radiation) in shades of gray and precipitation rate in rainbow colors. Courtesy: Center for Ocean-Land-Atmosphere Studies
As sophisticated as today’s climate models are, one critical component continues to hamper their effectiveness: clouds. Those white puffs of water vapor hovering overhead are computationally complex, requiring resources that even today’s most powerful supercomputers are hard-pressed to see through.

A recent massive attempt to resolve the climatic effects of clouds, Project Athena: High Resolution Global Climate Simulations, has just wrapped up a six-month intensive experimentation period, consuming 70 million CPU-hours and generating more than 900 terabytes of data using Athena, a Cray XT4 system at the National Institute for Computational Sciences (NICS), a TeraGrid partner.

Besides explicitly modeling cloud systems, Project Athena featured hundreds of weather prediction model simulations that sought to replicate the climate of the late 20th century, and to predict the impact of CO2 emissions on the Earth’s climate in the final decades of the 21st century. Researchers aimed to prove that enhanced resolution in climate simulations increases the accuracy of climate models.

“The ultimate goal of these simulations was to explore the possibility of revolutionizing climate and weather prediction, taking advantage of a large computing resource,” says Jim Kinter of the Center for Ocean-Land-Atmosphere Studies, and principal investigator in the project.

Two suites of simulations—one using an operational weather prediction code from the European Centre for Medium-range Weather Forecasts (ECMWF), and the other using the University of Tokyo’s NICAM model, a code that represents the global atmosphere at cloud-system resolving scales—were run to test one hypothesis, namely that simulating the climate system with low-resolution features and approximating clouds rather than including them explicitly impedes the accuracy of the model, while high-resolution features and explicit clouds enhance overall accuracy.

Having the entire Athena system for six months allowed the team to study numerous phenomena at unprecedented scales, as low as 7 kilometers in the case of the cloud-system-resolving model. For comparison, the U.S.’s National Weather Service currently uses a 35-kilometer model for global weather prediction.

In total, the ECMWF model was used for over 175 years of simulation at various resolutions, and the cloud-system-resolving NICAM model simulations consisted of eight northern hemisphere summers (May 21–August 31).

So does the use of explicit clouds rather than approximate clouds improve the models? Yes and no. The explicit cloud model produced excellent simulations of individual tropical cyclones and did very well on mean precipitation outside the tropics. However, when it came to the average precipitation in the deep tropics, the model produced “serious errors,” according to Kinter, noting that tropical thunderstorms were modeled especially poorly. The problem with the tropical precipitation simulation in NICAM, he said, is most likely the grid size, despite the enhanced resolution. “Ultimately, we probably need something as high resolution as a one-kilometer grid,” adds Kinter.

The global atmospheric circulation simulations, made using the numerical weather prediction model, likewise produced some interesting findings. In an effort to gauge future climate scenarios, Project Athena simulated the last 30 years of the 20th and 21st centuries, which confirmed some long-held fears.

For example, assuming CO2 levels continue to increase, the model indicates definitively that snow cover decreases at high altitudes in the future, which could lead to droughts in certain parts of the world. It also confirmed the need for more refined models—the outcomes of the higher resolution models (16 kilometers) seem to be more accurate than those at lower resolutions (125 kilometers).

“Project Athena also has demonstrated that dedicated supercomputing resources, such as the ones available in TeraGrid, can greatly increase scientific productivity on large projects. In our case, we achieved at least a factor of four increase in productivity,” says Kinter.

For more information: http://wxmaps.org/athena/home
Grant #s: NSF: 0830068, 0957884

Tropical cyclone intensity distribution, expressed as fractional frequency, as a function of maximum surface wind speed. The black bars are for the observed distribution. The colored bars are distributions from the ECMWF IFS model simulations. The inset shows an expanded view of the tail of the distribution. Courtesy: Center for Ocean-Land-Atmosphere Studies

Jim Kinter, Center for Ocean-Land-Atmosphere Studies

Tropical Computing—Literally

TeraGrid 2010
Asking “What If?” About H1N1

TeraGrid-based epidemiological modeling helped policymakers evaluate strategies for responding to the H1N1 flu epidemic.

Spread of H1N1 in the Washington, DC area—From the epidemiological modeling by Shawn Brown and colleagues, this graphic shows infected individuals per square mile, coded by color (increasing from blue to red), at the peak of the epidemic. Courtesy: Shawn Brown, PSC
The 2009 H1N1 flu epidemic raised many questions for public-health officials they hadn’t faced as seriously before:

• Should schools be closed? If yes, when and for how long?
• With a limited amount of vaccine, what groups—children, elderly, caregivers—should be vaccinated first?
• What about antivirals? Given limited supplies, what communities should get these relatively new medications and in what quantity?

During 2009, two National Institutes of Health MIDAS (Models of Infectious Disease Agent Study) research groups—one in Pittsburgh, one in Texas—relied on TeraGrid resources and applied two different, but complementary approaches to model the H1N1 outbreak. Their results, produced in real time during the epidemic, informed health care decision-makers locally, nationally and internationally. The MIDAS program helps health officials prepare for outbreaks by using computational tools to mimic how infectious disease spreads through populations.

Lauren Ancel Meyers, a MIDAS scientist at The University of Texas at Austin, used TACC’s Lonestar system to model H1N1 transmission within and among U.S. cities. Her model optimized choices for how to distribute the U.S. stockpile of antiviral medication, roughly 50 million doses. She presented her results and consulted with officials at BARDA (the U.S. Biomedical Advanced Research and Development Authority), with the U.S. Centers for Disease Control and Prevention in Atlanta, GA and the British Columbia Centre for Disease Control.

Brown and his colleagues consulted with the Allegheny County Health Department and health officials for the state of Pennsylvania as well as BARDA, the U.S. Department of Homeland Security, and the President’s Council of Advisors on Science and Technology.

https://midas.psc.edu
Grant #: NIGMS MIDAS 1U54GM088491-0109
Zeolite database is a potential mother lode of better materials

Data Mining New Materials

A visualization of a hypothetical zeolite structure from a database of 2.7 million zeolite-like materials. Courtesy: Michael Deem, Rice University
Zeolites are used to make everything from gasoline and asphalt to aquarium filters, laundry detergent and medical-grade oxygen. As useful as they are, however, nature has never been generous in supplying the silicate minerals with a porous Swiss-cheese-like structure used to speed or catalyze common chemical reactions on an industrial scale.

For decades, chemists relied on about 50 naturally occurring zeolites; during the past half century, researchers have bolstered the catalog to about 200 with the addition of synthetic varieties.

Recently, TeraGrid resources have opened what should become a monsoon-like deluge of new zeolites with potential, among other things, for saving energy and helping to address climate change and global warming.

Michael Deem of Rice University and David Earl of the University of Pittsburgh have used TeraGrid systems to identify millions of potential new zeolites by searching computationally for properly configured, hypothetically stable structures. Their database, two decades in the making, now contains 2.7 million unique structures for possible zeolites. It became publicly available in 2009 through a website and was highlighted in a *Journal of Physical Chemistry* cover article.

“We think it is a good first step,” Deem says. “The hope is that by studying the database we and others will find structures more efficient, for example, in terms of energy inputs or in waste byproducts.”

Deem and Earl have used resources from TeraGrid partners Purdue University, University of Chicago-managed Argonne National Laboratory, the National Center for Supercomputing Applications at the University of Illinois, the San Diego Supercomputer Center, and the Texas Advanced Computing Center. At Purdue, jobs were tailored to run in a distributed computing pool of nearly 30,000 processors from idle office, student computer lab and other machines. At one point, the pool was able to sustain a pace of 2,000 runs per hour. The project has completed 11.4 million jobs over 5.7 million computer hours in the pool since 2006.

In oil refining, for example, zeolites are essential catalysts in refining applications. But for most of these applications, only one useful zeolite is known. The new database of hypothetical zeolite structures could allow researchers to identify materials with dramatically improved function, leading to substantial energy efficiency improvements in the processing of oil.

The database already is being used by researchers at the University of California, Berkeley, who are looking for new materials to use in carbon sequestration, one possible tool to address global warming. Another potential application is improved hydrogen gas storage, which might be useful for greener hydrogen fuel cell vehicles or residential-based power plants.

Deem and Earl use statistical techniques to screen materials at an atomic scale in their search for zeolite-like structures.

“The work entails hundreds of simulations to examine a structure and requires far more computing power and data storage than would be available on any one campus,” Earl says.

For more information: www.mwdeem.rice.edu
Grant #s: TG: TG-MCA05S015; DOE/BES: DE-FG02-03ER15456
For further information: www.teragrid.org

TeraGrid Science Highlights 2010 was produced by the TeraGrid External Relations team, led by Elizabeth Leake, (UChicago-TG) and included: Trish Barker (NCSA); Bill Bell (NCSA); John Cobb (ORNL); Aaron Dubrow (TACC); Jim Ferguson (NICS); Warren Froelich (SDSC); Kay Hunt (Purdue); Joseph Insley (UChicago/Argonne); Scott Jones (ORNL); Carolyn Peters (UChicago/Argonne); Michael Schneider (PSC); Daphne Sieferth-Herron (IU); Faith Singer-Villalobos (TACC); Kristen Sunde (LONI); Marijke Unger (NCAR); Shandra Williams (PSC); Jan Zverina (SDSC).

Contributing writers/editors: Bill Bell (NCSA); Aaron Dubrow (TACC); Warren Froelich (SDSC); Kay Hunt (Purdue); Scott Jones (ORNL); Greg Kline (Purdue); Elizabeth Leake (TG); Michael Schneider (PSC); Daphne Sieferth-Herron (IU); Faith Singer-Villalobos (TACC); Kristen Sunde (LONI); Jan Zverina (SDSC).

Design: CarltonBruettDesign

The selection of Science Highlights for publication

Each year, the TeraGrid External Relations team publishes this booklet in an effort to showcase research accomplishments supported by TeraGrid resources and services. Stories are collected from each of the resource provide (RP) sites and from the annual reporting process. With help from TeraGrid’s Science Director, stories are selected that reflect one, or more, of the following qualities:

1. Potentially transform research in a particular domain.
2. Demonstrate the use of several TeraGrid resources across multiple RP sites.
3. Represent research conducted at a single RP—each of the eleven RP sites is represented.
4. Highlight work of individuals who are typically under-represented in high-performance computing (HPC).
5. Illuminate projects in fields of study that are typically under-represented in HPC.
6. Demonstrate TeraGrid’s impact—research that couldn’t have been accomplished without it.
7. Collaboration with other grids, international partners, business, and industry.

The Education, Outreach, and Training (EOT) team publishes the Science Highlights’ sister publication to showcase TeraGrid’s EOT activities each year. This year, the production of both publications is being led by ER and EOT team members from the San Diego Supercomputer Center (SDSC). The booklets are shared with researchers and educators at professional conferences and workshops. Further, the NSF Office of Cyberinfrastructure provides them to members of the Legislature in an effort to raise awareness about TeraGrid’s impact, thereby emphasizing the importance of continued funding of our nation’s cyberinfrastructure.
TeraGrid Resource Providers:

Indiana University (IU)
Louisiana Optical Network Initiative (LONI)
National Center for Atmospheric Research (NCAR)
National Center for Supercomputing Applications (NCSA)
National Institute for Computational Sciences (NICS)
Oak Ridge National Laboratory (ORNL)
Pittsburgh Supercomputing Center (PSC)
Purdue University (Purdue)
San Diego Supercomputer Center (SDSC)
Texas Advanced Computing Center (TACC)
University of Chicago/Argonne National Laboratory (UChicago/Argonne)

Sponsored by the
National Science Foundation’s Office of Cyberinfrastructure