

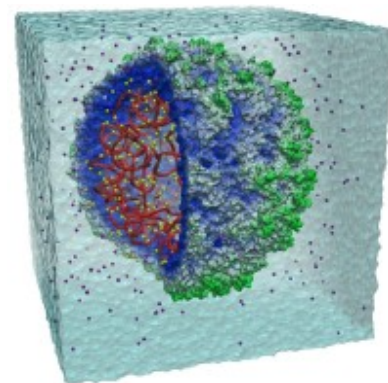
Harnessing Supercomputers to Model Life

For the first time, researchers have visualized the changing atomic structure of a virus by using powerful computers to calculate how each of the virus' one million atoms interacts every femtosecond, or one-millionth-of-a-billionth of a second. The NSF-funded simulation revealed key physical properties of satellite tobacco mosaic virus, a simple, plant-infecting virus. A better understanding of viral mechanisms helps researchers design improved strategies to combat viral infections in plants, people and other animals.

Led by Klaus Schulten of the University of Illinois at Urbana-Champaign, the research team tapped high-performance computing power at the National Center for Supercomputing Applications to run the simulation. Still, it took about 100 days to generate just 50 nanoseconds of virus activity.

Ultimately, scientists will generate longer simulations from bigger biological entities; but to do so, they need the next generation of supercomputers. NSF is currently devising a national strategy to give scientists and engineers the resources needed to tackle their most computationally intensive research problems.

For more on the first virus simulation, see ["Supercomputer Maps One Million Atoms of a Complete Virus in First Simulation of a Life Form."](#)



Researchers at the University of Illinois at Urbana-Champaign completed the first all-atom simulation of satellite tobacco mosaic virus. Credit: University of Illinois at Urbana-Champaign's Theoretical and Computational Biophysics Group.

New "Voice over Internet Protocol" Test Bed Will Improve Security



A University of North Texas-led collaboration is developing a geographically distributed, secure test bed to analyze Voice over Internet Protocol (VoIP) vulnerabilities. VoIP allows people to make toll-free phone calls over the Internet. Some 24 million U.S. households are predicted to use the new technology by 2008. The test-bed project aims to identify security issues and solutions before damage is done. Credit: Nicolle Rager Fuller, NSF.

NSF has issued four awards totaling \$600,000 to a University of North Texas-led, multi-university collaboration to develop a geographically distributed, secure test bed to analyze vulnerabilities in Voice over Internet Protocol (VoIP) -- an increasingly popular technology that turns audio signals into digital data that can be transmitted over the Internet.

The three-year project will investigate voice spam prevention (VoIP systems can be spammed like email), attacks on networks and Internet resources that render them unavailable (denial of service), quality of service, and 911-service dependability. The test bed will also be used to discern security holes arising from VoIP interacting with conventional phone networks.

VoIP allows users with a computer and a standard Internet connection to make toll-free calls anywhere in the world. Companies such as Vonage and AT&T are aggressively deploying the technology, and one study predicts some 24 million U.S. households will be using VoIP by 2008.

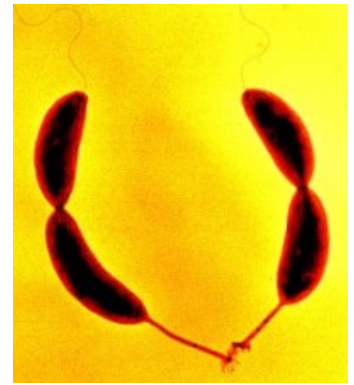
The project also includes researchers and resources at Columbia University, Purdue University and the University of California-Davis. The team is committed to disseminating its findings throughout academia, industry and government, giving all technology developers guidelines for preventing security breaches. See ["Collaboration Will Investigate Vulnerabilities of Rapidly Growing Internet Phone and Multimedia Systems"](#) for more details.

Sticky Bacterium Produces Natural Superglue

The glue that one species of water-loving bacterium uses to grip its surroundings may be the strongest known natural adhesive. If the material proves easy to mass produce, it could have applications in medicine, marine technology and other areas.

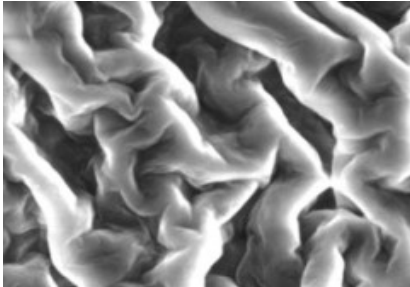
Researchers at Indiana University and Brown University studied how much force they needed to tug the tiny, stalked *Caulobacter crescentus* off a glass plate. The bacteria grip with a force of five tons per square inch -- equivalent to the downward force exerted by three cars balancing on a spot the size of a quarter.

While the researchers do not yet know if the substance is the strongest glue on Earth, it is stronger than cyanoacrylate superglues found on store shelves and may be rivaled by only a few synthetics. Funding for this study came from the Division of Materials Research in the Mathematics and Physical Sciences Directorate. For more information, see "[Waterproof Superglue May Be Strongest in Nature.](#)"



Two cells of an aquatic bacterium attach to a surface, and each other, by their glue-secreting "holdfasts." The holdfast is the structure at the tip of the stalk, a thin extension of the cell. Credit: Yves V. Brun, Indiana University.

Microcapsule Offers Potential Drug Delivery Technology



An electron micrograph shows the outer membrane of a microcapsule, which wrinkles and collapses when its temperature drops, forcing out its contents. The tool may someday deliver medicine or cosmetics. Credit: Sahraoui Chaieb, Univ. of Illinois at Urbana-Champaign.

A tiny, temperature-sensitive capsule could prove to be a major breakthrough for both medicine and cosmetics. Sahraoui Chaieb -- a physicist and NSF CAREER awardee -- together with his colleagues at the University of Illinois at Urbana-Champaign crafted tiny, hollow capsules from lipids that wrinkle and collapse when cooled below body temperature. The collapsed capsules, ranging in size from 10 to 100 micrometers across, squeeze out chemicals in a controlled manner.

The capsules are in the earliest stages of development and not yet ready for medical use, but the researchers are discussing potential applications of the technology with a cosmetics company. Before the capsules can deliver medicine, the researchers say they must develop a mechanism to cool the tiny pills without endangering surrounding body tissues. For more information, see "[Micro Pills Could Deliver Drugs on Demand.](#)"

DID YOU KNOW?

NSF Nurtures Small Companies with Big Ideas

NSF piloted the [Small Business Innovation Research \(SBIR\) and Small Business Technology Transfer \(STTR\) Programs](#) over 20 years ago. Since then, the programs have spread to 10 federal agencies. Coordinated by the Small Business Administration, these agencies collectively support over \$2 billion in innovation research each year. Such programs have nurtured small companies into major market leaders, such as Symantec, Qualcomm, Sensant (now part of Siemens), Vivisimo, Displaytech and Aurora Flight Sciences. NSF awarded more than 300 SBIR/STTR grants in FY 2005, for a total investment of \$100 million.

The success of the SBIR/STTR programs has led to their replication around the world as nations strive to find new ways to compete in the global, technology-enabled, innovation economy. See the [NSF Fact Sheet](#) for more SBIR/STTR breakthroughs.



Emergency response personnel test FAST-ACT, a material that absorbs hazardous substances. Kansas State University chemist Kenneth Klabunde devised nano-engineering techniques, which resulted in FAST-ACT's development. Then with NSF-SBIR support, Klabunde founded NanoScale Materials, Inc. to commercially produce this new family of substances. Credit: NanoScale Materials, Inc., NSF.

Catlett Touts TeraGrid for All of Science and Engineering



The NSF-supported TeraGrid was fully deployed in Sept. 2004 as a national computing and data storage network that combines resources from eight partner sites. By accessing the TeraGrid, researchers from all fields of science and engineering are applying high-performance computing power to their studies. Recently, we had a little data exchange of our own with TeraGrid Director Charlie Catlett.

Why is it called the “TeraGrid?”

“Tera” is a prefix meaning “trillion.” By connecting some of our nation’s most powerful computing resources, we created a system that can perform 100 trillion floating point operations per second—or 100 teraflops. In comparison, a high-end desktop computer today performs in the range of a few billion flops. So, the TeraGrid is in some sense like 50,000 desktop computers working together.

Is the TeraGrid a unique resource?

The TeraGrid is the most powerful open computational facility in the world. While there are similar “grid” projects, TeraGrid offers the unique advantage of tightly coupled, distributed computing resources for scientific discovery that would not be possible within a single computer center.

Another unique aspect of TeraGrid is the Science Gateways Initiative. Rather than assuming that scientists will adapt their work to fit our systems, the TeraGrid accommodates pre-existing tools, databases and collaborative sites that scientists in their respective fields have already built.

Science Gateways are plugged directly into the TeraGrid, making TeraGrid much more inviting and productive for researchers. Users can access TeraGrid through systems to which they are already accustomed while the computing infrastructure functions transparently in the background.

How many researchers are using the TeraGrid?

As of early this month, we provided computational support for well over 2,000 researchers working on more than 1,000 scientific projects.

What’s next for TeraGrid?

We have several challenges ahead of us. The first is to really make these new “grid” computing tools and services easier to use so that researchers can focus on science rather than computers.

We are also concentrating on making sure that our information management, analysis, and data movement infrastructure can continue to support a new generation of data-centric science as the volume of data grows by an order of magnitude.

Lastly, we are carefully considering the future workforce. Today’s students can now engage in scientific discovery using TeraGrid computing resources. When they enter the workforce, we want them familiar with authentic science -- including advanced computing tools.

Do you consider yourself a computer geek?

I’m such a computer geek that I used a GPS to track our location on a cruise during spring break. I’ve already meshed the track with pictures on a Google map.

It’s not technology that I’m a geek about – it’s what you can do with it. I’ve worked in supercomputing for 23 years now. And though I enjoy the technology, the real lessons I’ve retained have to do with understanding how scientists, educators and students do their work with these tools, and what makes things easier for them to stay productive.



Charlie Catlett,
TeraGrid Director

NSF IN THE NEWS

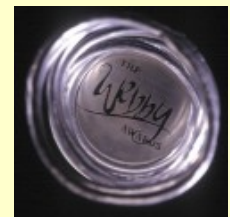
Climate-Monitoring Satellites Successfully Launched Into Orbit

-- *Associated Press (04/16/06)* -- Six weather satellites successfully reached orbit Saturday, launching their five-year mission to monitor hurricanes, climate change, and space weather. The \$100 million effort is jointly funded by Taiwan and several federal agencies in the United States, including the National Science Foundation.

Chimps Could Hold HIV Key -- *Rocky Mountain News (04/10/06)* -- Aurora, Colo.-based Evolutionary Genomics earlier this year received its second \$500,000 National Science Foundation grant to study the differences between chimpanzee and human DNA that make the former resistant to AIDS and the latter receptive to it. It is believed that chimps were carriers of HIV for at least a million years before it passed to humans.

NSF Web Site on the Shortlist for Top International Honor

The NSF Web site has been nominated for a 2006 Webby Award, the leading international honor for Web sites. The NSF site is one of five finalists in the government category.



NSF redesigned its site in 2005 to better serve the general public and the science and education communities, with a greater emphasis on visual richness and user-friendliness. As a Webby nominee, the site is also eligible to win a People’s Voice Award. Voting is open to the public from April 11 to May 5 at <http://peoplesvoice.webbyawards.com>.

A Statement from the Director -- "Racing for the Future"

Without exception, a chance to venture outside of Washington D.C. brings new insight. I recently had the opportunity to visit Mauldin Elementary School in Simpsonville, South Carolina with Congressman Bob Inglis. The time I spent with a class of fifth-grade engineers reminded me that enthusiasm is contagious. The fifth-graders got me enthusiastic about the world of engineering all over again!

I had the opportunity to witness the culmination of a 13-week, student immersion in engineering, design, propulsion, physics and metrics. Four-member teams of anxious fifth-graders raced their balloon-propelled model cars as part of the "A World in Motion" program. The teams had designed their cars completely from recycled materials, plastic pipes, paper clips and push-up cylinders, for example.

The construction project not only changed attitudes about math and science, it also changed outlooks. Before construction began, the students were asked to describe what engineers do on the job. The most common responses were: drive a train or take care of a building like their school. At the conclusion of the project, they were again asked about a career in engineering. Their answers were dramatically different... from designing cell phones and space shuttles to ensuring that the water we drink is safe.

The opportunity for a hands-on project generated great excitement and competition among the groups. They fine-tuned their cars -- and their skill -- through trial and error and observation. And most importantly, they all discovered that science is fun and provides limitless possibilities. For these students, the project opened a whole new understanding of what they can do with knowledge in science and technology -- a truly transformational classroom experience.



Students prepare their model

"A World in Motion," now in its 16th academic year of distribution, makes learning math, science and engineering fun. Funded by the Society of Automotive Engineers International (SAE), the curriculum joins together teachers, students and volunteer practicing engineers and scientists to explore physical sciences. For example, BMW -- the area's largest employer -- chipped in a few techno-savvy expert volunteers to participate in Mauldin Elementary School's program.

I am both pleased and proud that the National Science Foundation helped start this program years ago via grants. The good idea has taken on a life of its own, and now reaches more than two million students. According to SAE, the two main ingredients in the curriculum were fun and a challenge -- a lesson in the value of engagement for policymakers, administrators, teachers, and parents alike.



Bement visits with students of Mauldin Elementary School

Café Scientifique

"A Place to Eat, Drink and Talk About Science"

When: **First Tuesdays of the Month**
6:00-8:00PM

Details: **Free and open to public.**
No science background required!
Limited seating - first come, first seated.

Sponsored by the National Science Foundation
Inputs and questions welcome to mhanson@nsf.gov
or sgoforth@nsf.gov.

In the name of making science more accessible, NSF sponsored its first Café Scientifique on April 4, 2006. For the inaugural event, more than 120 guests -- scientists, students, and the general public -- joined astrophysicist Michael Turner for food, drink and conversation about the origins of the universe. Dr. Turner fielded questions on everything from string theory to philosophy.

The next Café will be **Tuesday, May 2**, at **The Top of the Hill** (aka Pour House), 319 Penn. Ave., SE (2nd floor), from 6-8 p.m. Our speakers will be journalist **Kathy Sawyer**, author of "**The Rock From Mars**," and NASA scientist **Mike Meyer**, on the topic "**Are We All Martians? What We Know, Don't Know and Want to Know About Mars.**"

Meet speakers whose expertise spans the sciences -- and who can talk in plain English -- at future monthly events. Stay posted for details!



The National Science Foundation (NSF) is an independent federal agency that supports fundamental research and education across all fields of science with an annual budget of nearly \$5.58 billion. NSF funding reaches all 50 states through grants to roughly 1,700 universities and institutions. Each year, NSF receives about 40,000 competitive requests for funding and makes about 10,000 new funding awards. The NSF also awards over \$400 million in professional and service contracts yearly. Contact [NSF's Office of Legislative and Public Affairs](#) for more information, to unsubscribe, or for permission to reuse newsletter images.