CASC: Coalition for Academic Scientific Computation

Academic Innovation in Advanced Computing

Accelerating U.S. Competitiveness

Contents

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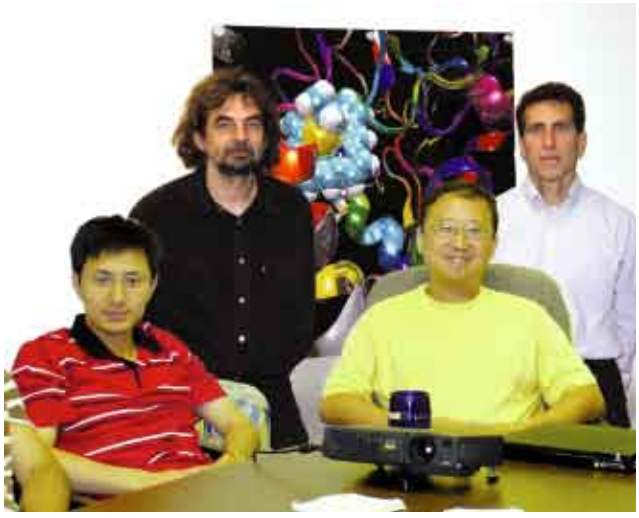
About the Cover

High-performance computers play a critical role in helping scientists understand the detailed workings of proteins – the workhorse molecules that participate in virtually every process within our cells. This insight is critical to the development of new therapeutic measures to treat disease and improve the quality of life. Pictured on the cover is the active site of the enzyme (protein) Cytochrome P450, which plays a crucial role in the metabolism of drugs and toxins in our body.

Cytochrome P450 was modeled on a 13 Teraflop Linux cluster at the University at Buffalo's Center for Computational Research (CCR) using Density Functional Theory. The calculations predict changes in the active site geometry upon binding of the protein Putidaredoxin, key to the function of Cytochrome P450.



The calculations were carried out by Doctors Marek Freindorf and Thomas R. Furlani of the CCR (top row), and by Doctors Jing Kong and Yihan Shao of Q-Chem, Inc., Pittsburgh, Pennsylvania (bottom row). The resulting image was created using VMD [Visual Molecular Dynamics] and then rendered on a visualization cluster using POV-Ray [Persistence of Vision Raytracer] by Adam Koniak of the CCR. Photo illlustration by Gail Bamber.

About CASC

Founded in 1989, the Coalition for Academic Scientific Computation (CASC) is an educational 501(c)(3) nonprofit organization with 49 member institutions representing many of the nation's most forward thinking universities and computing centers. CASC advocates the use of the most advanced computing technology to accelerate scientific discovery critical to national competitiveness, global security, and economic success. CASC also promotes advanced technology as an essential tool in the development of a skilled and diverse 21st century workforce to fuel the nation's technological leadership.

The mission of CASC is to:

- disseminate information about the value of high performance computing and advanced communications technologies;
- provide an expert resource for the Executive Office of the President, the Congress, and federal agencies, as well as state and local government bodies; and
- facilitate information exchange within the academic scientific computation and communication community.

Computational science has become the third pillar of scientific enterprise, a peer with traditional methods of physical experiments and theoretical investigations. Coalition members provide high performance computing (HPC) resources, massive data storage facilities, visualization environments, and software. Connected via high-capacity optical networks, cyberinfrastructure enables large-scale, long-term, multi-disciplinary networking and information technology R&D, and innovative research at the frontiers of science. By applying advanced technology, CASC members extend the state of the art to achieve scientific, technical and information management breakthroughs beyond imagination, positioning the U.S. at the forefront of the 21st century knowledge economy.

This brochure provides a snapshot of the research contributions of CASC members – from simulating new pharmaceuticals to modeling climate change, and from detecting brain aneurisms to developing new energy technologies. More detailed descriptions of each CASC members' contributions to discovery, innovation, and learning are available at:
www.casc.org/members.html CASC

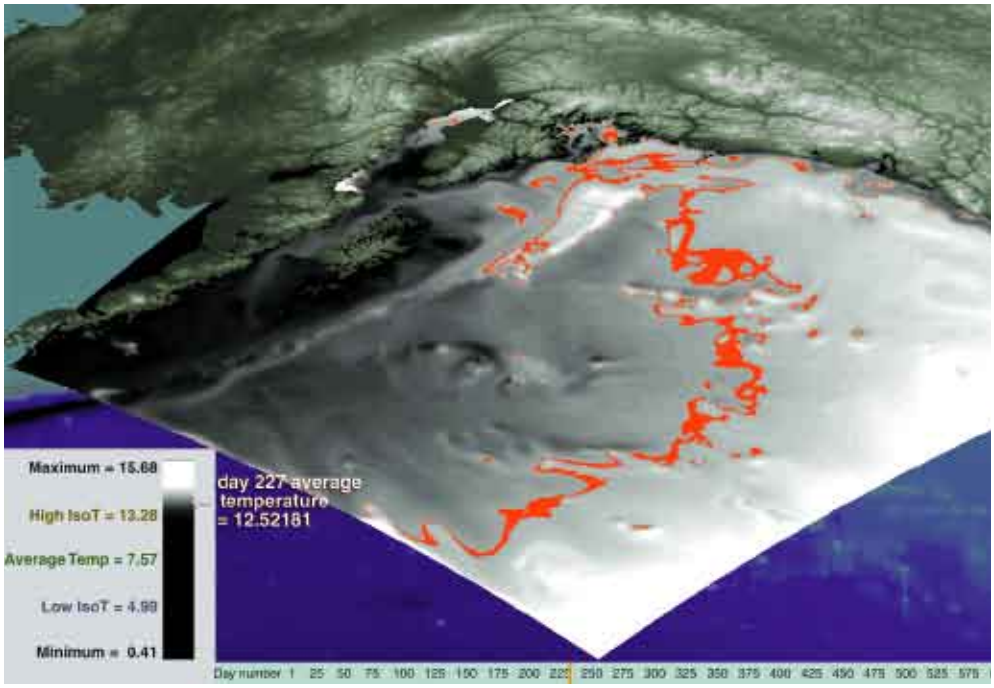
This 3D visualization produced by the Pittsburgh Supercomputing Center from simulations by the Center for Analysis and Prediction of Storms at the University of Oklahoma, Norman, captures time evolution of an F5 tornado. With wind speed over 260 MPH, it is the most intense tornado ever simulated. Features that can be seen in the visualization, such as the twisting vortex and unstable wave patterns, agree well with real tornados, and detailed analysis of the visualization provides new understanding of tornado genesis and dynamics.

Academic Innovation in Advanced Computing
Accelerating U.S. Competitiveness

The Evolution of Academic Cyberinfrastructure

In the 1960s, the National Science Foundation (NSF) first recognized the need for investments in advanced scientific computation by funding a number of computing centers on university campuses. The NSF made a bold leap forward in the mid 1980s, funding the NSF Supercomputer Centers program, which operated from 1985 to 1997. The centers were instrumental in pushing the envelope of hardware and software, as well as advancing the frontiers of network infrastructure, leading to further advances in computing and groundbreaking grid projects such as today's TeraGrid and Open Science Grid. Similarly, early, substantial and sustained investments by the Department of Energy (DOE) and the Defense Advanced Research Projects Agency (DARPA) fostered pivotal network research and critical computing capabilities that continue today with the DOE's Advanced Scientific Computing Research program and DARPA's High Productivity Computing Systems program. CASC members continue to be at the forefront in advancing such national research initiatives, as well as major state-funded information technology programs.

In the 20th century, the United States competed in the space race. In the 21st century, we compete in the information race, which takes place at the speed of light. Optical networks link advanced computing architectures in this race for solutions to the most daunting problems facing humanity today.

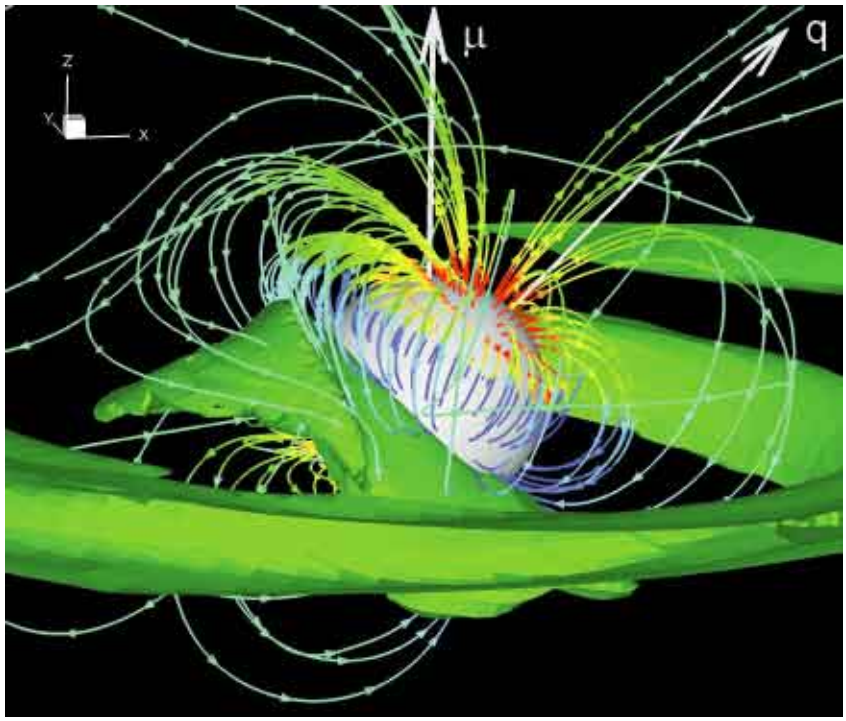


With visualization by the Arctic Region Supercomputing Center at the University of Alaska Fairbanks, sea surface temperature (in °C) of the northern Gulf of Alaska show seasonal warming and cooling. The red band indicates where the ocean is warmer than average over a two-year period.

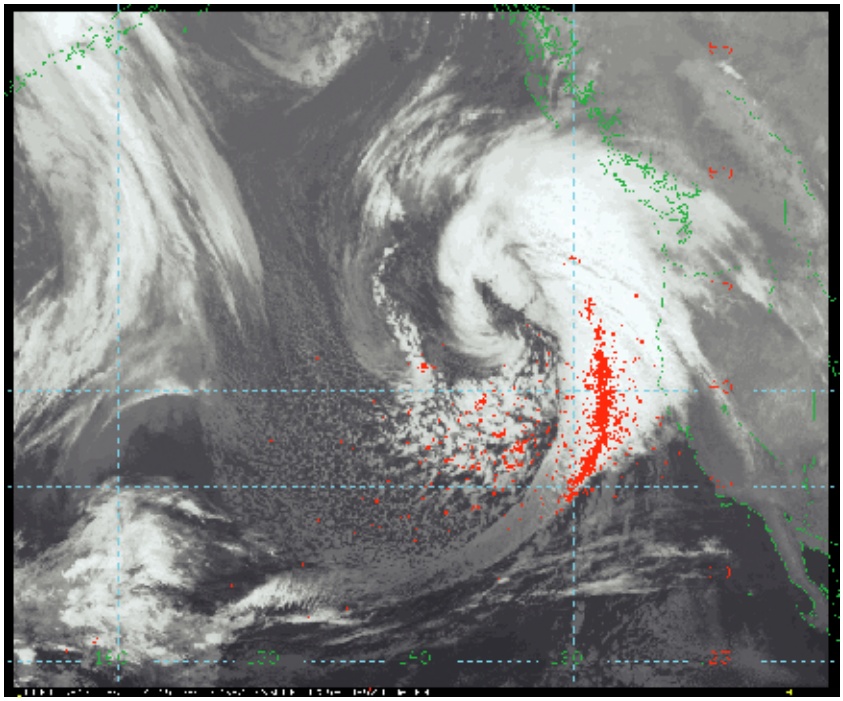
From the far reaches of space to inner workings of molecules, discoveries resulting from NSF investments in research and education enable the United States to remain at the forefront of science and engineering knowledge and also enhance the nation's economic strength in the face of global competition.

–2006 in Review, NSF

CASC members are driving advancements in a range of critical research initiatives – from bioinformatics to healthcare, from nanotechnology to the environment, and from cybersecurity to global security. Moreover, our members are investing in the nation's human capital by building awareness of how information technologies can educate and train citizens, from K-12 students to working professionals. A sampling of these initiatives is provided in the sections that follow. CASC



Astrophysicists are employing the high-speed, parallel computers at the Cornell Center for Advanced Computing to enable 3D modeling of the complicated flows of ionized matter drawn into rotating magnetized stars. These models are essential to understand how stars are born, live, and die.



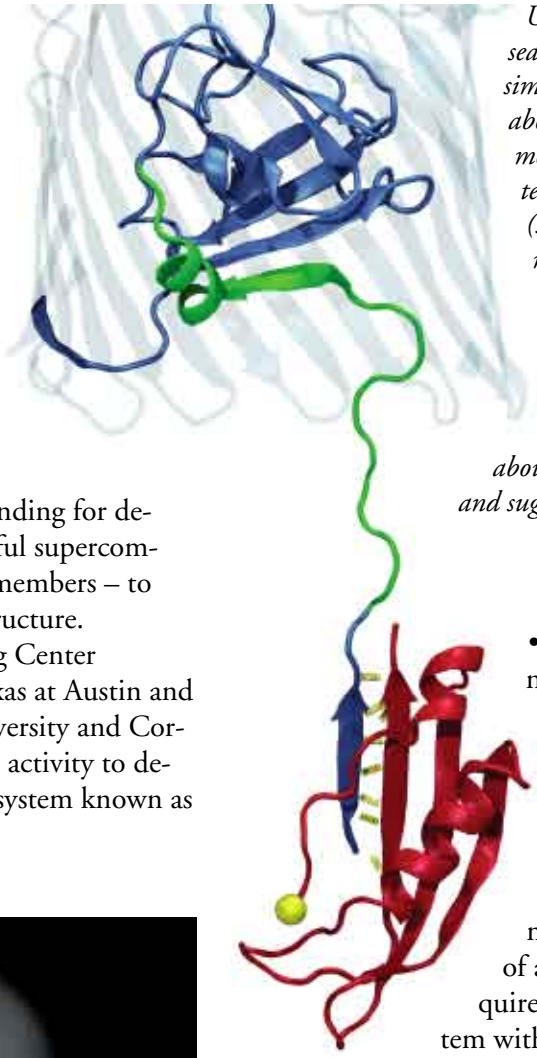
Researchers at the University of Hawaii use advanced computation and visualization to understand strong winter storms and lightning patterns within those storms. At right is a visualization of a strong winter storm over the eastern Pacific. GOES-10 satellite images are overlaid with long-range data on locations of lightning strikes (the red dots) to show the pattern of lightning within the storm.

Accelerating the Nation's Research Enterprise

Over the last few years, rich information technology environments, known as *cyberinfrastructure*, have emerged that aggregate distributed computing resources, data repositories, visualization and analytical tools, and people, all linked together by software and high performance networks to improve research productivity and enable breakthroughs not otherwise possible.

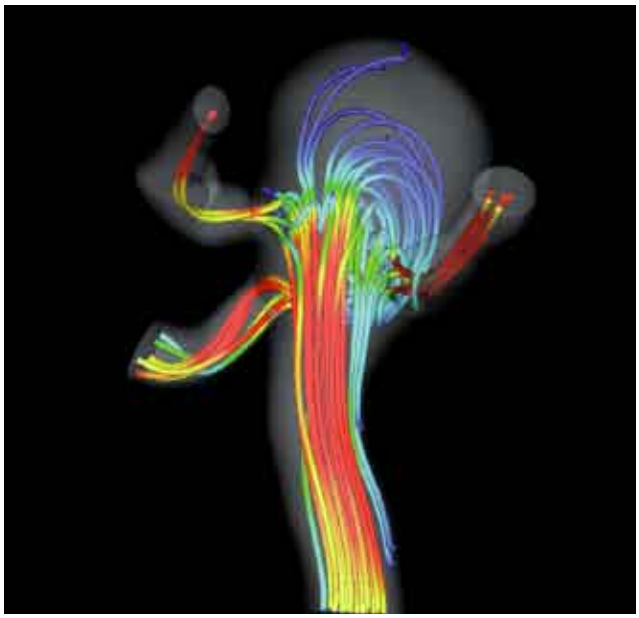
The NSF recently announced funding for deployment of the world's most powerful supercomputers – all implemented by CASC members – to further fuel the nation's cyberinfrastructure.

- The Texas Advanced Computing Center (TACC) at the University of Texas at Austin and its partners at Arizona State University and Cornell University are engaged in an activity to deploy and operate a leading-edge system known as "Ranger" in late 2007.



University of Illinois researchers used supercomputer simulations to test hypotheses about how bacteria take up large molecules. They modeled the interaction of the protein TonB (shown in red) and outer membrane proteins (in green and dark blue), using Indiana University's Big Red and NCSA's Abe systems via the TeraGrid. Their simulations eliminated one hypothesis about the transport mechanism, and suggested new ones.

- The University of Tennessee at Knoxville Joint Institute for Computational Science (JICS) and its partners at Oak Ridge National Laboratory, TACC, and the National Center for Atmospheric Research are part of a five-year project to acquire an extremely powerful system with a peak performance of just under one petaflop.



New imaging capabilities are invaluable in medical research moving it beyond the detection of the anatomical presence of disease. This is a frame from a cardiovascular simulation series using the Lonestar system at the Texas Advanced Computing Center. The image shows an aneurism of a cerebral artery. Warm colored streamlines represent regions of high velocity magnitude – areas where the blood is flowing fastest – while cool colors represent regions of low velocity magnitude, where blood is flowing at a slower rate because an aneurism has constricted blood-flow.

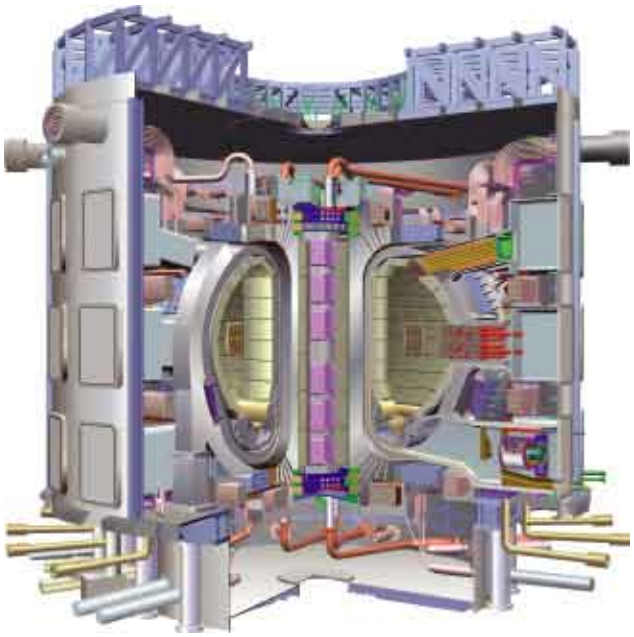
[E]nvironments and organizations, enabled by cyberinfrastructure, are increasingly required to address national and global priorities, such as understanding global climate change, protecting our natural environment, applying genomics-proteomics to human health, maintaining national security, mastering the world of nanotechnology, and predicting and protecting against natural and human disasters, as well as to address some of our most fundamental intellectual questions such as the formation of the universe and the fundamental character of matter.

– NSF Blue Ribbon Advisory Committee report,
Revolutionizing Science and Engineering through Cyberinfrastructure

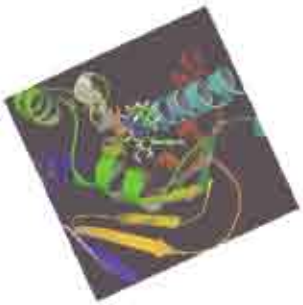
- The National Center for Supercomputing Applications (NCSA) will operate a petascale computer it calls "Blue Waters," which is 500 times more powerful than today's typical supercomputers. This 'leadership-class' system is expected to go online in 2011.

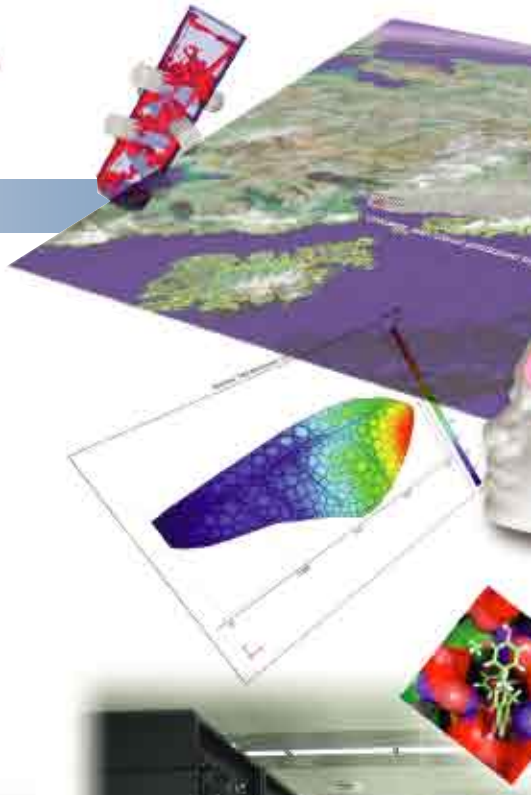
The projects below are representative of the forward-thinking, national cyberinfrastructure initiatives in which CASC members play a significant leadership role.

- NSF's TeraGrid is the world's largest, most powerful and comprehensive distributed cyberinfrastructure for open scientific discovery, involving eleven resource partner sites. Using ultra high-performance network connections, the TeraGrid integrates leadership-class computers, data resources and tools, and high-end experimental facilities. It currently supports more than 1,000 projects and over 4,000 researchers geographically spanning the entire United States.
- The National Institutes of Health (NIH) Biomedical Informatics Research Network (BIRN) integrates biomedical research efforts across key research centers throughout the U.S. BIRN is a consortium of 25 universities and 33 research laboratories that participate in testbed projects on brain imaging of human neurological disorders. By enabling earlier and more accurate identification of brain disorders via a shared forward-looking infrastructure, it promises tremendous potential for diagnosis and treatment of diseases such as Alzheimer's and Parkinson's.
- The Open Science Grid (OSG) is working to satisfy the ever-growing computing and data management requirements of scientific researchers, especially collaborative science requiring high-throughput computing. Participating research communities gain low-threshold access to a greater number of resources than they could individually afford. OSG is a consortium of software, service, and resource providers, as well as researchers. Funded by the NSF and DOE, OSG resources are forging new discoveries to improve understanding the very essence of matter. CASC



ITER is a major international magnetic fusion project to demonstrate the scientific and technological feasibility of fusion energy, the power source of the sun and the stars. The ITER machine is based on the tokamak concept, in which a hot gas is magnetically confined in a torus-shaped vessel. Physicists and engineers throughout the U.S. are working on ITER and using resources at the National Energy Research Scientific Computing Center and Oak Ridge National Laboratory.





Sustaining the Nation's Competitive Edge

With IT transforming economies worldwide, now more than ever the United States must remain vigilant in advancing discovery and innovation through continued and increasing investment in a strong national research infrastructure. High performance computing is one of America's greatest competitive strengths. It provides opportunities for scientific breakthroughs allowing U.S. industry to maintain an edge in R&D, to pursue "high-risk, high-payoff" ideas, and to speed proof-of-concept of new products to the global marketplace.

For more than two decades, CASC member universities and centers have been the core of our nation's research enterprise. We're helping U.S. industry sustain its global leadership in the evolution of information and communications technologies as well as spurring innovation and productivity across all sectors. Americans are the most productive

CASC members are helping U.S. businesses tap into the world's most powerful computers to help them innovate and compete globally.

Images courtesy of:

- *Arctic Region Supercomputing Center*
- *National Center for Supercomputing Applications*
- *Indiana University/National Institutes of Health*
- *Ohio Supercomputer Center*
- *Pittsburgh Supercomputing Center*
- *Renaissance Computing Institute*
- *Texas Advanced Computing Center*
- *Texas A&M University Supercomputer Center*
- *University of Hawaii*

While the United States clearly is the global NIT [Networking and Information Technology] leader today, we face aggressive challenges from a growing list of competitors. To maintain — and extend — the Nation's competitive advantages, we must further improve the U.S. NIT ecosystem — the fabric made up of high-quality research and education institutions, an entrepreneurial culture, strong capital markets, commercialization pathways, and a skilled NIT workforce that fuels our technological leadership.

—President's Council of Advisors on Science and Technology, 2007

workers in the world. One reason for this is the speed at which U.S. companies develop and implement new network and information technologies.

Whether a micro-cap or blue chip company, our industrial partners are reducing the time and effort required to bring a product to market by tapping into the cutting-edge computational resources as well as the scientific and technical expertise of CASC members. As strategic partners we are working to ensure that the United States remains the world's premier place for innovation, to create high-paying jobs and a comfortable standard of living, as well as increased security for our citizens. CASC

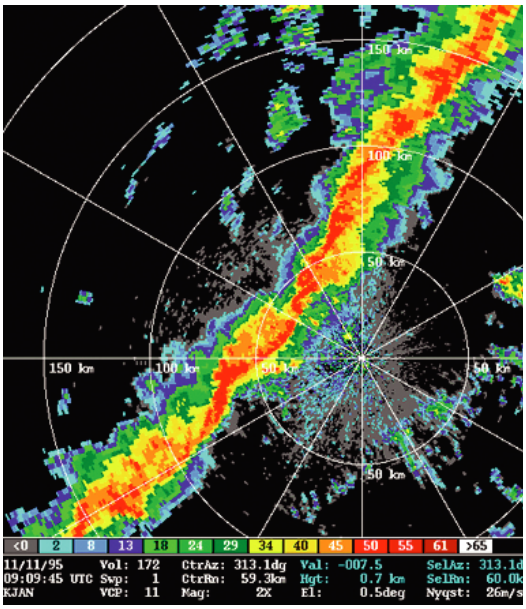
Driving Discovery and New Knowledge

Federal and state investments in HPC have spurred innovation and created a national fabric to accelerate research. Whether too hazardous to study in a laboratory or too time consuming or expensive to solve by traditional methods, this rich networked information technology infrastructure is enabling the multi-disciplinary, collaborative research that leads to rapid and systematic advancements for the nation's economic prowess and our quality of life.

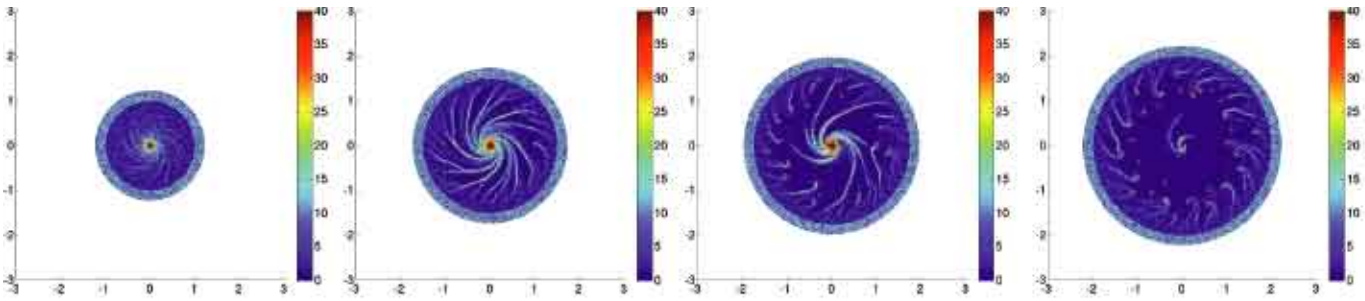
- Thirty years ago many supercomputers were at work defending the lives of citizens in the service of national security. Today's supercomputers are driving innovation and defending lives in entirely new ways. Modern supercomputers are analyzing the structure of proteins and the function of biological pathways to help scientists fight disease and improve human health.
- America faces the dual challenge of reducing national health care costs while providing affordable, quality services for its citizens. High performance computing is increasingly important to achieving both goals. CASC institutions are at the forefront of medical research, using their resources to expand knowledge, increase collaboration, and improve health care delivery. As a result, medical providers routinely employ

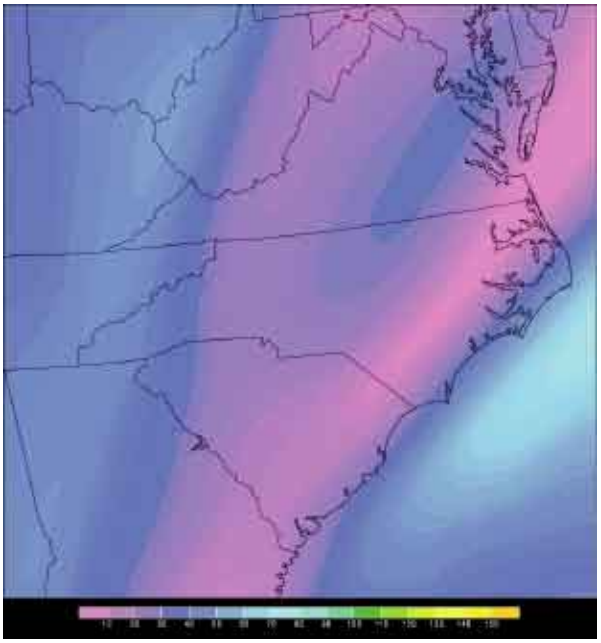
We must build and strengthen the third pillar of the triad of discovery if we are to probe the deepest secrets of Nature and reap the technical, economic, and social benefits such under-standing will yield.

***—DOE Office of Science, Occasional Paper on* The Challenge and Promise of Scientific Computing**



Purdue's Rosen Center for Advanced Computing and Information Technology is distributing high-resolution, real-time NEXRAD Level II radar data which are widely used in university research and teaching programs in the fields of atmosphere sciences and climatology, hydrology, agriculture, transportation, and economics. A web portal enables researchers to analyze data using TeraGrid resources.

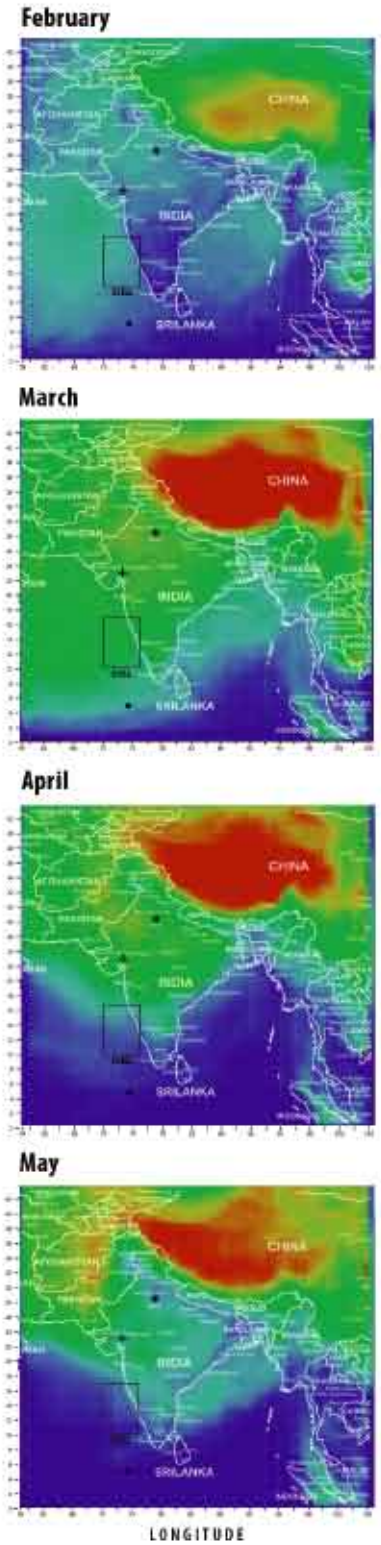




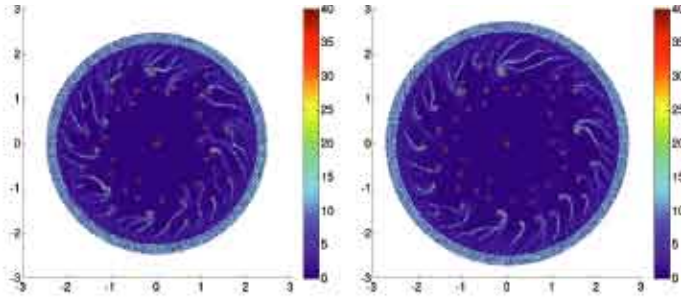
With computational resources available at the Renaissance Computing Institute, meteorologists are able to plot wind magnitudes in knots along the Carolina coast to improve weather forecasts and hurricane predictions. The highest winds, shown in bright aqua, are southeast of Cape Lookout, and the lowest winds appear in bright pink.

high bandwidth networks for real-time, remote diagnostics. Federal support for research that applies advanced computer technology to health care delivery is proving a sound investment.

- Scientists working to predict severe weather have one simple goal: to determine the likely occurrence and path of tornadoes and hurricanes quickly and accurately enough for people in affected areas to get out of harm's way. CASC members are hard at work improving the capabilities of weather models, expanding the capabilities of the supercomputers and grid computing systems to make real-time predictions, and save lives. CASC



Many of the Earth's environmental challenges are not confined by international borders. Using resources from the Ohio Supercomputer Center, U.S. researchers collaborated with colleagues around the world to further understand the broader impact of industrial development in China.



Proteus mirabilis is a bacterium which can cause severe urinary tract infections and other diseases. It is well-known for its ability to swarm over hard surfaces and form a variety of spatial patterns. Researchers at the University of Minnesota are using mathematical modeling to understand how the bacterium colonizes surfaces – an important first step toward devising treatments that eradicate it. The cell colonization visualization sequence is over a three hour period.

The data deluge represents an opportunity to advance U.S. leadership in science and technology, and harnessing it has become a national priority. More robust NIT capabilities are needed to fully exploit large-scale data resources.

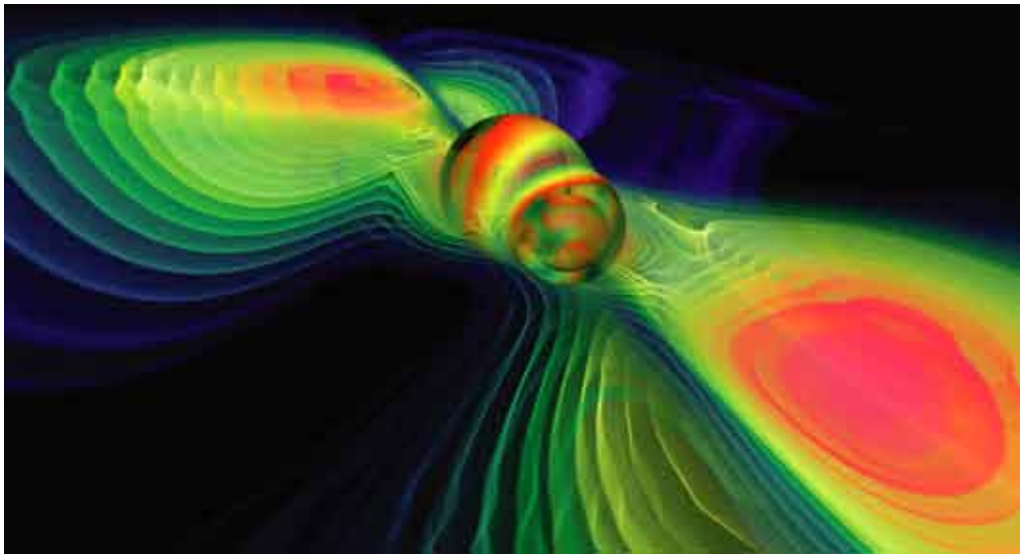
—President's Council of Advisors on Science and Technology Committee Report,
Leadership Under Challenge: Information Technology R&D in a Competitive World 2007

Data, Data Everywhere

The image shows USC Shoah Foundation Institute's Visual History Archive search interface. For preservation purposes, USC will begin the process of re-digitizing the videotaped interviews in a lossless, compressed format; when completed the archive will use over 4 petabytes of online storage.

Today most new information is 'born digital,' and results in a data deluge. The overwhelming masses of digital data available via network-connected devices present a critical data-management problem. Creating new tools vital to collecting, organizing, analyzing, storing, and reusing data is a high priority for CASC members. Powerful science gateways provide a logical interface for scientists to access supercomputers and data storage resources required to support today's leading-edge scientific discovery and innovation.

While managing large complex data sets is a well-known challenge in the hard sciences, it is also a significant challenge among scholars from the social sciences and humanities. For example, the Sloan Digital Sky Survey (SDSS) – which includes millions of x-ray, infrared, and visible light images of over a hundred million celestial objects – requires over 40 terabytes of information. In comparison, the Shoah Foundation Institute's Visual History Archive at the University of Southern California is a compilation of nearly 52,000 videotaped interviews of Holocaust survivors and other witnesses, collected in 32 languages and from 56 countries. A digital copy of the archive created by the Institute for general access uses over 175 terabytes of online storage. CASC



Researchers from the Louisiana State University Center for Computation & Technology are collaborating with both the Albert Einstein Institute and the Zentrum für Informationstechnik Berlin (ZIB) in Germany to further understanding of Black Hole collisions and about gravitational waves. Researchers use these visualizations to try and detect the presence of these waves to prove the last part of Einstein's Theory of Relativity.

People are the fundamental resource ...

—President's Council of Advisors on Science and Technology Committee Report,
Leadership Under Challenge: Information Technology R&D in a Competitive World 2007

Inspiring the Next Generation of IT Professionals

Today CASC members are accelerating the capacity of supercomputers, networks, and software for the next generation of America's information technology ecosystem. In addition, we are developing the workforce of tomorrow to utilize, program and administer *their* cyberinfrastructure.

Our members are actively engaged in education, outreach and training programs designed to increase the number of students pursuing advanced degrees in computer science and engineering. And, we're training students in the multi-disciplinary teamwork needed to solve complex, real-world problems. Our members are leading programs designed to broaden the participation of new communities to ensure that America's best and brightest includes minorities and women who are contributing to and reaping the benefits of the 21st century knowledge economy.

CASC member outreach programs start at the elementary school level and continue through graduate education and lifelong learning for established professionals. CASC

CASC members are educating and training the next generation of innovators from all of America's diverse cultures. At the Center for Excellence and Equity in Education at Rice University, students discover that robotics really is fun.

The University of New Mexico (UNM) is helping the Navajo Nation make use of grid computing for educational delivery and economic development. Pictured are staff of the Navajo Technical College beta testing a back haul network connection for a satellite campus. This project is also part of the TeraGrid partnership.

In a virtual classroom collaboration with Elizabeth City State University (a minority serving institution), CASC members are helping to prepare students for a future in cyberinfrastructure-enabled science, the knowledge based economy, and the scientific professoriate.

Accelerating the Agenda of the U.S. Federal and State Governments

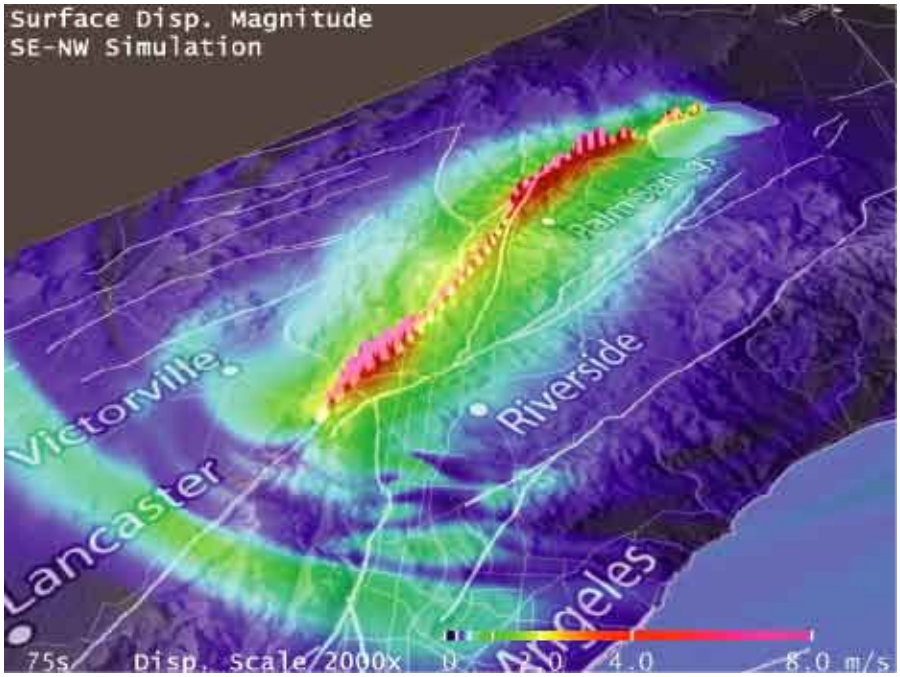
CASC members develop partnerships with federal and state government entities to contribute to strategic national goals. A representative list appears below:

U.S. Federal Government

Department of Commerce
  National Oceanic and Atmospheric Administration
Department of Defense
Department of Education
Department of Energy
  National Nuclear Security Administration
Department of Homeland Security
Environmental Protection Agency
Institute of Museum and Library Services
Library of Congress
National Aeronautics and Space Administration
National Archives and Records Administration
National Endowment for the Humanities
National Institutes of Health
National Science Foundation

Federal Advisory Committees

NSF Computer Information Sciences and Engineering Advisory Committee
NSF Office of Cyberinfrastructure Advisory Panel
President's Council of Advisors on Science and Technology



Researchers at the Southern California Earthquake Center and the San Diego Supercomputer Center modeled the tremors that would rattle Southern California if a 230-kilometer section of the San Andreas fault ruptured and produced a magnitude 7.7 earthquake. It is the largest and most detailed simulation of the region to date, creating more than 40 Terabytes of data.

CASC Members

Advanced Research Computing, Virginia Tech, Blacksburg, VA

Advanced Computing Center for Research and Education, Vanderbilt University, Nashville, TN

Advanced Scientific Computation Center, Northeastern University, Boston, MA

Arctic Region Supercomputing Center, University of Alaska, Fairbanks, AK

Arizona State University, Tempe, AZ

Boston University Center for Computational Science, Boston, MA

Center for Academic Computing, The Penn State University, University Park, PA

Center for Advanced Academic Computing, University of Michigan, Ann Arbor, MI

Center for Advanced Computing Research, California Institute of Technology, Pasadena, CA

Center for Computation & Technology, Louisiana State University, Baton Rouge, LA

Center for Computational Research, University at Buffalo, Buffalo, NY

Center for Computational Sciences, University of Kentucky, Lexington, KY

Center for High Performance Computing, University of New Mexico, Albuquerque, NM

Center for High Performance Computing, University of Utah, Salt Lake City, UT

Clemson University, Clemson, SC

Computer and Information Technology Institute, Rice University, Houston, TX

Cornell University Center for Advanced Computing, Ithaca, NY

East Carolina University, Greeneville, NC

Georgetown University, Washington, DC

Georgia Institute of Technology, Atlanta, GA

High Performance Computing Center, Texas Tech University, Lubbock, TX

Indiana University, Bloomington, IN

Maui High Performance Computing Center, University of Hawaii, Honolulu, HI

Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN

Mississippi State University, Mississippi State, MS

National Center for Atmospheric Research, Boulder, CO

National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign, Champaign, IL

National Energy Research Scientific Computing Center, Berkeley, CA

National Supercomputing Center for Energy and the Environment, University of Nevada, Las Vegas, NV

NDSU Center for High Performance Computing, North Dakota State University, Fargo, ND

Oak Ridge National Laboratory Center for Computational Sciences, Oak Ridge, TN

Ohio Supercomputer Center, Columbus, OH

OU Supercomputing Center for Education and Research, University of Oklahoma, Norman, OK

Pacific Northwest National Laboratory, Richland, WA

Pittsburgh Supercomputing Center, Pittsburgh, PA

Purdue University, West Lafayette, IN

Renaissance Computing Institute, Chapel Hill, NC

Rensselaer Polytechnic Institute, Troy, NY

San Diego Supercomputer Center, La Jolla, CA

Texas A&M University Institute for Scientific Computation, College Station, TX

Texas Advanced Computing Center, University of Texas at Austin, Austin, TX

Texas Learning and Computation Center, The University of Houston, Houston, TX

University of Florida, Gainesville, FL

University of Iowa, Iowa City, IA

University of Miami, Miami, FL

University of Nebraska, Omaha, NE

University of South Florida, Tampa, FL

University of Southern California Information Sciences Institute, Marina del Rey, CA

Utah State University, Logan, UT

The country that out-computes will be the one that out-competes.

– Council on Competitiveness

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