ABOUT THE COVER IMAGE: The impact of BP’s massive oil spill on coastal areas, resulting from the April 20, 2010 explosion of the Deepwater Horizon offshore oil-drilling rig in the Gulf of Mexico, was simulated by researchers using the Ranger supercomputer at the Texas Advanced Computing Center (TACC), of The University of Texas at Austin. With an emergency allocation of 1 million computation hours from the National Science Foundation TeraGrid project, five researchers ran high-resolution models of the Louisiana coast to track the oil (shown as yellow lines) through complicated marshes, wetlands, and channels to determine how the oil would spread in those environmentally sensitive areas. The researchers received satellite images of the spill from the Center for Space Research at UT Austin, and downloaded meteorological data from the National Centers for Environmental Protection (NCEP) – a division of the National Weather Service – every six hours. They combined the data into a 72-hour forecast with a resolution of 50 meters. For each model run, the ADCIRC (Advanced Circulation Model for Oceanic, Coastal, and Estuarine Waters) simulation used 4096 compute cores on Ranger for three hours (equivalent to 512 days of computation on a standard computer); the group performed between one and four model runs per day. The five researchers, shown below, are (from left to right): Clint N. Dawson, head of the Computational Hydraulics Group at the Institute for Computational Engineering and Sciences (ICES) at The University of Texas at Austin; Rick Luettich, head of the Institute of Marine Sciences at the University of North Carolina at Chapel Hill; Johannes Westerink, professor of civil engineering at the University of Notre Dame; and two members of the TACC staff who did the visualization work, Adam Kubach and Karla Vega.
The Coalition for Academic Scientific Computation (CASC) was founded in 1989, when information technology, high performance computing, and the internet were coming of age. CASC is an educational 501(c)(3) nonprofit organization. Its mission encompasses the following:

- disseminating information about the value of high performance computing and advanced communications technologies
- providing an expert resource for the Executive Office of the President, the Congress, and federal agencies, as well as state and local government bodies
- facilitating information exchange within the academic scientific research, computation and communication communities

CASC is dedicated to the use of advanced computing technologies to accelerate scientific discovery that will improve national competitiveness, global security and quality of life, and provide economic benefit. Our members are committed to developing a diverse and skilled 21st-century workforce, to support regional economic growth in science and technology and fuel the nation’s technological research.

Today, CASC’s 67 members in 36 states and the District of Columbia are among the nation’s most innovative research universities, high performance computing centers and institution-partnered Federal laboratories. CASC members (listed on pages 14 and 15) provide high performance computing resources, massive data storage facilities, visualization environments, analytical instruments, software and expertise.

The world has changed dramatically over the past two decades. Our members continue to be committed to advancing our nation’s research and education enterprise. For more than two decades, CASC members have enabled detailed computer simulations, advanced data analyses, and breakthrough discoveries.

This brochure provides snapshots of the research contributions of CASC members – from modeling global climate to understanding blood cholesterol, from visualizing the formation of galaxies to analyzing efficient combustion. More detailed descriptions of each CASC member’s contributions to discovery, innovation, and learning are available at: www.casc.org/members.html

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Powerful new computer software released by the National Center for Atmospheric Research (NCAR) allows scientists to study climate change in unprecedented detail. This image, taken from a larger simulation of 20th-century climate, depicts several aspects of Earth’s climate system. The color scales at bottom and right show sea surface temperatures and sea ice concentrations. The figure also displays sea level pressure and low-level winds. Such simulations, produced by the NCAR-based Community Climate System Model, can also depict precipitation and other weather events. Companion software, recently released as the Community Earth System Model (CESM), will enable scientists to study the climate system in even greater complexity. The models are jointly supported by the Department of Energy (DOE) and NCAR’s sponsor, the National Science Foundation (NSF); this image is © copyright University Corporation for Atmospheric Research.
Computational science has become the third pillar of scientific enterprise, a peer with traditional methods of physical experiments and theoretical investigations. It has revolutionized the way science and engineering are done, becoming indispensible to our nation’s welfare, competitiveness, and standing in the international scientific community.

In the 1960s, the National Science Foundation (NSF) funded the first computing centers on several university campuses. Two decades later, NSF took a bold leap by funding the Supercomputer Centers program, which operated from 1985 to 1997. Those centers not only pioneered the design of both advanced computing hardware and software, but also advanced the frontiers of network infrastructure, leading to groundbreaking collaborative grid projects such as today’s TeraGrid — which brings together leadership-class resources at eleven CASC member sites — and the Open Science Grid.

Early major and sustained investments by the Department of Energy (DOE) and the Defense Advanced Research Projects Agency (DARPA) fostered the development of pivotal network and computing capabilities. The pioneering work of the two agencies continues with the DOE’s Advanced Scientific Computing Research (ASCR) program and DARPA’s High Productivity Computing Systems program.

The resulting "cyberinfrastructure" — America’s broad collection of computing systems, data acquisition and storage systems, and visualization environments, linked by high-speed networks and supported by expert professionals — is today one of our country’s most important national assets. CASC members have contributed much in designing our nation’s cyberinfrastructure, and continue to be at the forefront.

High performance computing allows unprecedented modeling of systems so complex they were long regarded as intractable: systems such as global climate and weather prediction, global flows of energy and money, cosmology, natural disasters, manufacturing, genetic diseases, and drug design. With the advent of exascale computing — systems a thousand times more powerful than the fastest of today’s (petascale) supercomputers — researchers will be able to tackle scientific and engineering problems of even greater complexity.

The extraordinary value of computational science arises from its interdisciplinary collaborations: It draws not only from mathematics, computer science, engineering and technology, but from all scientific disciplines. Moreover, it addresses research challenges that cross traditional boundaries and are essential to America’s daily life.

A black hole is a massive body that has collapsed to become so dense that not even light can escape. Whether an individual star or a supermassive black hole in the center of a galaxy, it grows by accreting gas from rings of gas and other matter in orbit around it. Two University of Virginia astronomers — John F. Hawley and Kris Beckwith — explore how magnetic fields drive one powerful feature of accretion disks: astrophysical jets, which can fire matter hundreds, thousands, even millions of light years away. Simulations conducted on a variety of TeraGrid systems, including the Intel 64 cluster Abe at the National Center for Supercomputing Applications (NCSA), revealed that the strength and longevity of these astrophysical jets are highly sensitive to the overall configuration of the magnetic field. Pictured here is a quadruple magnetic field topology, showing gas densities in an accretion disk (dark blue indicates low gas density, and dark red indicates high gas density).
Our energy and transportation choices and the greenhouse gases our technologies emit will have lasting impact on the Earth, as shown in this simulation of the world in 2030, looking east from the Pacific Coast of the United States. The image summarizes the results based on a climate model from the National Oceanic and Atmospheric Administration’s (NOAA) Geophysical Fluid Dynamics Laboratory. The vertical bars reflect the emissions of heat-trapping gases in a given location; the colors depict temperature increases in degrees Fahrenheit. The darker green represents no change in temperature; the yellows represent an increase of 5°F; the lighter red an increase of 7°F; and the deep red an increase of fully 14°F. Alex Betts and Bob Patterson at the National Center for Supercomputing Applications (NCSA) Advanced Visualization Laboratory, in coordination with Donald Wuebbles, Nobel laureate and professor of atmospheric sciences at the University of Illinois at Urbana-Champaign, produced this visualization to understand potential impacts to both ecosystems and societies resulting from human-related emissions.

The main ingredients in soaps and detergents are surfactants, chemical agents that wet a surface and change the properties of a liquid. Surfactants are also important for drug-delivery systems. Mixtures of surfactants, water, and other molecules are exceptionally challenging to model, because they aggregate themselves into three-dimensional structures called micelles that can trap materials, the way soap traps dirt so both can be washed away. In these images by Alex Kohlmeier, a team from four institutions (Iowa State University’s Ames Laboratory, the University of Michigan, the University of Pennsylvania, and Temple University’s Institute for Computational Molecular Dynamics) modeled a time sequence of the assembly process of one type of surfactant—shown here as the molecules with two green tails—using NCSA’s Abe and Lincoln supercomputers. First, the individual molecules assembled into what look like “hands” (upper left) and then combined into a larger three-dimensional structure (moving clockwise from upper right to lower right) before ending up as a bilayer (the zipper-looking structure at lower left).
In order to build the most accurate computational models — especially for applications where human lives are at stake, such as the modeling of severe storm systems — many disciplines in science and engineering have become increasingly data-driven.

As the world becomes more instrumented, most new information is ‘born digital.’ Massive volumes of digital data are collected, integrated and interpreted via modeling, visualization, and data mining — sometimes in real time. Detailed data lead, in turn, to new and better models and hypotheses, accelerating discovery and innovation.

For researchers and businesses alike, however, the volume of data from network-connected devices is becoming overwhelming. The data deluge, often likened to a tidal wave or tsunami, is now posing critical data-management challenges: handling data inflow from sensors or experiments, managing data outflow from simulation models, and storing information by means that both protect its integrity and preserve long-term access to it.

But data-intensive computing requires more than just storing and moving large volumes of data. It requires imaginative new architectures. The complexity of massive data sets, as well as the increasing diversity of data flows, render the traditional model of a computer data center inadequate for modern scientific research. A new infrastructure model is needed to enhance our capabilities for managing and interpreting the data, in order to accelerate discovery and innovation.

A high priority for CASC members is creating both new infrastructure and new tools for collecting, organizing, analyzing, storing, and reusing data. Many CASC members are pioneering the development of vital and innovative new data management tools, which are changing the way multi-investigator, multi-disciplinary research teams manage and analyze massive data sets.

“Since 2003, digital information makes up 90 percent of all information production, vastly exceeding the amount of information on paper and film.”

A Report of the National Science Foundation Task Force on Cyber Science and Engineering, National Science Foundation, 2010

For solar energy to become truly cheap, not only must we be able to capture incoming sunlight, but also to store solar energy in chemical bonds for use when the sun isn’t shining. Storage of captured solar energy requires a transport material for delivering separated charges (such as electrons) to catalytic sites; it also requires an efficient catalyst for using the delivered charge to carry out a chemical reaction that stores the harvested solar energy. All aspects of this process are being investigated at the Energy Frontier Research Center (EFRC) at the University of North Carolina. One potential transport material, under investigation by Shubin Liu, Cynthia Schauer, and Thomas J. Meyer, is an organic molecular system called a chiral dual porphyrin complex. In this visualization, created to predict the molecular system’s chemical reactivity, red regions have extra electrons available for donation and blue regions are areas where more electrons can be accepted. Such visualizations help facilitate understanding of the movement of charges in the catalytic process.
Figuring out how a protein can enter a human cell without destroying the cellular membrane is vital to the design of pharmaceutical drugs that could use that protein as a delivery tool. This visualization, by Margaret Cheung and her student Qian Wang at the Texas Learning and Computation Center of the University of Houston, shows a penetratin protein interacting with a dodecylphosphocholine (DPC) micelle; the micelle, a ball-like dump of molecules that forms when a detergent is added to water, mimics the properties of human cellular membranes. In the image, the micelle is the large network of molecules in blue and red. The yellow and brown blobs are the two key amino acids in the penetratin protein for binding to the micelle. Computational models reveal that the two amino acids actually pack together to allow the penetratin to slip through the membrane.

“Digital preservation is a societal challenge because information is a vital resource in our knowledge economy.”

High performance computing is one of America’s greatest competitive strengths. Federal and state investments in high performance computing have created a national fabric to ignite innovation, create rapid and systematic advancements in research and industry, strengthen the economy, and improve our quality of life. Some problems are too hazardous or large-scale to study in a laboratory, or too time consuming or expensive to analyze by traditional experimental methods. But our computational prowess allows scientists to explore “high-risk, high-payoff” ideas, and helps industry to speed proof-of-concept of new products into the global marketplace.

Visualization, methods of data analysis, and simulations have become the principal means of understanding vast data sets in many areas of science and engineering. According to a 2009 assessment of international capabilities in simulation-based engineering and science by the World Technology Evaluation Center (WTEC), visualization is revolutionizing research and technology in all fields.

It is transforming the way disease is treated and surgery is performed, the way patients are rehabilitated, and the way we understand the brain. It is altering the way materials and components are designed, developed, and used in all industrial sectors. And it is aiding in the recovery of untapped oil, the discovery and utilization of new energy sources, and the design of sustainable infrastructures.

CASC members are driving advancements in research that ranges from bioinformatics to healthcare, from nanotechnology to the environment, and from cybersecurity to global security. For example, since 2004, the Blue Collar Computing™ program of the Ohio Supercomputer Center (OSC) has provided smaller businesses with modeling and simulation tools that allow for the virtual development of new and improved products. OSC provides advanced modeling and simulation resources, hardware, training, software, and expertise to commercial clients, allowing them to meet their economic and competitiveness needs by improving the time, quality, and cost of product and service development.

“...virtually all businesses — large and small — that adopt HPC (high performance computing) consider it indispensable for their ability to compete and survive.”

Benchmarking Industrial Use of High Performance Computing for Innovation, Council on Competitiveness, 2008

A team of researchers at Temple University’s Institute for Computational Molecular Science, led by Grace Brannigan, is changing the way scientists view cholesterol and anesthetics: specifically, that cholesterol may play an important role in enhancing the effectiveness of anesthetics. For years, cholesterol was thought only to be in the outer region of a structure called the nicotinic acetylcholine receptor (nAChR), which is important in transmitting signals to neurons and muscles. But in work that began at the University of Pennsylvania’s Center for Molecular Modeling with the help of the National Center for Supercomputing Applications (NCSA), supercomputer simulations indicate that the cholesterol molecules may be buried deep within the receptor. This work could lead to the design of anesthetics that are more powerful than the ones available today but with fewer side effects.
RS Vulpeculae is a double star system in which gas from a cool, orange sun-like star flows towards a hotter, brighter, more massive, but smaller, blue star. These images, by a team led by Mercedes Richards and Elena Slobovnov at Pennsylvania State University, represent three-dimensional velocity maps of the gas flow, based on actual stellar spectra acquired from Kitt Peak National Observatory in Arizona; the data were analyzed with tomography software similar to codes used in processing medical images. The top image shows a view partially above the orbital plane of the stars, with gas flowing around the blue star within the two magenta circles; the bottom image shows how the gas flows above and below the orbital plane (magenta line). The brightest gas is red, the faintest gas is green, and the solid red line simulates how gravity affects the gas flowing between the stars. These images suggest that the cool star’s magnetic field has an unexpectedly large effect on the movement of the gas.

Computer-aided drug design (CADD) is a promising means of developing antiviral drugs. A team led by computational and structural biologists Thomas Cheatham and Darrell Davis at the University of Utah is targeting the genetic material, or RNA, by which a virus copies itself inside cells. Specifically, they have for the first time determined the atom-by-atom structural details of a part of the hepatitis C virus RNA (red, white, and blue framework). Shown is a critical bulge on the viral RNA internal ribosomal entry site (IRES) sequence, which binds an antiviral chemical compound (yellow and blue), thereby inhibiting the RNA from replicating the hepatitis C virus. Because the viruses causing swine fever, foot-and-mouth disease, and other diseases also contain IRES sequences, structure-based CADD may help develop drugs targeting RNA for a range of viral diseases. Simulations were performed at the Pittsburgh Supercomputing Center and National Institute for Computational Science.

Advanced animated simulations, such as this one by Gil Bohrer at The Ohio State University, help researchers to study forest wind flows and understand the complex interactions between the atmosphere, trees and soil, as well as their impact on the wider climate. This frame, from a simulation of a high-resolution atmospheric model, shows the treetop canopy as a lumpy green sheet and tree trunks as vertical brown lines. The wind is visualized as white streamlines representing the paths air follows. Humidity and temperature are represented by blue and red regions on the side and back “walls.” Using the computational power of the Ohio Supercomputer Center, the animation reveals that the location of strong updrafts, which eject moist warm air from the canopy to the atmosphere above, depends on the structure of the forest canopy. Those ejections are responsible for exchanging most of the water vapor and carbon dioxide between the canopy and the atmosphere.
Our nation's capacity to innovate hinges on retaining a skilled workforce, continually refreshed by students who are knowledgeable in science, technology, engineering and mathematics (STEM). As noted in the 2010 report *Rising Above the Gathering Storm, Revisited: Rapidly Approaching Category 5*, only four percent of our nation's workforce are scientists and engineers, yet they disproportionately create jobs for the other 96 percent. Innovation benefits not just the scientists, engineers, and entrepreneurs, but also the factory workers who build the new products, the advertisers who promote them, the truck drivers who deliver them, the sales professionals who market them, the consumers who buy them, and the maintenance people who service them.

Harnessing powerful new supercomputers for scientific discovery and engineering innovation, however, requires a greater grasp of the fundamentals of scientific computation than is now commonly taught in STEM programs, particularly in those that rely on a "black box" use of

> “Global competition increasingly requires that the U.S. make the necessary investments in science and engineering research and education.”
>
> Coalition for National Science Funding, 2010

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How fatigue weakens and cracks metals and their alloys is crucial in engineering, especially aerospace. Molecular dynamics, a computational method that models the forces and distances between atoms, can model materials at very small scales. This visualization of a “block” of pure aluminum measures 300 atoms wide, 40 atoms high, and 25 atoms deep. Aluminum is ductile, and under stress it makes internal nucleations — dislocations of atoms — before it actually cracks. The color scale spans from deep blue (fewest nucleations) to bright red (most nucleations). In the simulation, a force pulls the block vertically upward at the rate of 100 meters per second. This timestep in the sequence of images documents the instant nucleations joined to form a crack (black). Teresa Konopka, a sophomore majoring in aeronautical engineering at Rensselaer Polytechnic Institute in New York, ran the simulation in summer 2010 as part of a Research Experience for Undergraduates (REU) program under Douglas E. Spearot at the University of Arkansas.
commercial software packages. To become tomorrow’s computational scientists and engineers, today’s students need to master underlying concepts of modeling, programming, and “algorithmic thinking” critical to using computers in a scientific context. Many CASC members are actively meeting that need.

CASC members are dedicated to educating and training both today’s workforce and tomorrow’s thought leaders. From elementary school through high school, our members’ outreach programs ignite students’ curiosity and fascination with math and science.

Exemplary computational science courses, in-depth workshops, and summer institutes motivate university undergraduate and graduate students, as well as faculty and established professionals. CASC members also train our nation’s educators to incorporate the most sophisticated science and engineering research tools and approaches in their class rooms. Our members are leading programs designed to broaden the participation of groups who have been traditionally underrepresented in high performance computing, and developing programs for inspiring our current workforce to use advanced computation.

Antonio B. Rodriguez (blue shirt), of the University of North Carolina at Chapel Hill’s Institute of Marine Sciences, works with undergraduate and graduate students on a beach near Morehead City to set up and calibrate a LIDAR (Light Detection And Ranging) optical remote sensing unit to map the beach. The LIDAR unit collects topographic data in an effort to understand how storms, including hurricanes, affect beach erosion. This work is relevant to climate change research because predicted higher sea levels and stronger storms may mean greater erosion. Rodriguez and the students use the same unit to monitor the growth of oyster reefs (oysters are important to the North Carolina economy) and to measure the shoreline erosion of marshes.

Two undergraduate students work on the Remote Control Devices Project, a grant-funded undergraduate research effort by the Arctic Region Supercomputing Center of the University of Alaska Fairbanks. The project’s fundamental aim is to expose off-site students and teachers to the challenges of controlling robots remotely through a custom-designed, web-based interface. Multiple users can log in simultaneously, manipulate separate robots in the same environment, and work together to complete tasks and scenarios. Participants gain exposure to a work environment that is becoming increasingly important, such as in remote-controlled surgery, robotic repairs and inspections, and extraterrestrial and under-ocean exploration.

Each summer, the Center for Computational Research at the University at Buffalo holds the annual Eric Pitman Summer Workshop in Computational Science to encourage western New York high school students to develop skills and interest in computational science. High school sophomores, juniors, and seniors spend two intensive weeks at the New York State Center of Excellence in Bioinformatics and Life Sciences to learn computer programming and its application to problems in visualization, chemistry, and bioinformatics. Here a group is learning about the center’s visualization capabilities; the speaker is demonstrating the tiled display wall — which projects 15 million pixels in 88 square feet — in a virtual tour of the university’s north campus.
America faces many challenges and opportunities. These include reducing national health care costs while providing affordable, quality services for its citizens; understanding more about climate change and related disciplines; and designing new materials almost molecule by molecule to make manufactured products lighter, stronger, safer, more effective, and less expensive.

We’ve entered an era in which high performance computing is increasingly important in achieving these and other goals. For example, CASC institutions are at the forefront of medical research, using their resources to expand knowledge, increase collaboration, and improve personalized health care delivery. As a result, medical providers routinely employ high bandwidth networks for real-time remote diagnostics. Federal support for research that applies advanced computing and networking technologies to health care delivery is proving a sound investment.

While computationally intensive techniques have created successful three-dimensional popular movies such as *Avatar*, the same techniques are now extending far beyond the entertainment industry. Humans are innately visual creatures, with half our brains devoted to processing visual information. In computational terms, vision is by far our highest-bandwidth data path — and **visual data exploration is fundamental to our ability to interpret models and understand complex phenomena,** whether the goal is designing a jet fighter aircraft or a new nanomaterial.

The progression of visual presentation, game design, and game capabilities has created intense interest in marrying high performance computing with visualization technologies for serious and important goals, ranging from military training to scientific understanding. CASC members are leading the way in these areas.

“**Without visualization, discovery will not be possible.**”

Visualization and Knowledge Discovery: Report from the DOE/ASCR Workshop on Visual Analysis and Data Exploration at Extreme Scale, Office of Advanced Scientific Computing Research, Department of Energy, October 2007
The technical and cultural boundaries between modeling, simulation, and games are increasingly blurring...

The Rise of Games and High Performance Computing for Modeling and Simulation
Committee on Modeling, Simulation, and Games; Standing Committee on Technology
Insight — Gauge, Evaluate, and Review; National Research Council, 2010

Visualizing vector data — that is, quantities with both magnitude and direction in three dimensions, such as velocity — is important in many scientific fields. One application in geology is visualizing the time evolution of ground motion for an earthquake. Amit Chourasia and his colleagues at the San Diego Supercomputer Center have developed a novel representation to encode vector data using shape, color, size, and shading. Their interactive application called GlyphSea allows scientists to explore vector data by visualizing glyphs or symbols — in this case an ellipsoid, with a white dot on one pole indicating the leading edge of a vector and a black dot on the opposite pole indicating the trailing edge. This image is one time step from a simulation of a hypothetical point-source earthquake. The new visualizations clearly depict wave propagation through the earth (including P-waves and S-waves in three dimensions). GlyphSea is being used to explore realistic earthquake simulations as well as to study magnetic turbulence data from astrophysics simulations.

Combustion produces over 80 percent of the nation’s energy, but also a large percent of air pollutants. Robert Cheng and colleagues at Lawrence Berkeley National Laboratory (LBNL) developed a low-swirl burner for turbines and furnaces. Requiring no pilot light or moving parts, it is a nozzle fitted to the end of a fuel pipe. Inside the nozzle, airfoil-like vanes make the flow of fuel swirl and expand radially as it exits the pipe, creating a local stagnation region where a bowl-shaped flame can sit indefinitely. If enough swirl is added to hold the flame steady while not trapping any hot combustion products in a recirculation above the flame, it can burn lean with ultralow emissions. The simulation, by LBNL’s Center for Computational Sciences and Engineering and the National Energy Research Scientific Computing Center, is from a study of lean hydrogen-air mixtures, showing a cutaway profile of the concentration of OH molecules (which are produced and consumed at the flame). Red areas mark regions of intense combustion. Fine gray-blue vortex structures at the base of the flame mark turbulence.

Knowledge about how nature unites both the animal and the mineral to form such complex structures as mollusk shells and human bone is relevant for designing medical implants, drug delivery vehicles, and other applications for the replenishment of human tissue. In this snapshot of a molecular dynamics simulation from research conducted by Hendrick Heinz at the University of Akron and the Ohio Supercomputer Center, the central red, white and blue structure represents a peptide — a short protein strand (calcitonin, in this image) — that can form silicate structures under certain conditions. It is shown binding to the stepped surface of gold (yellow balls) in a water solution (the many small red and white elements). Heinz is examining several metals (including gold, mica, montmorillonite and a palladium-gold bimetal) to determine how they might bind with a number of minerals (including calcitonin, ettringite, tricalcium silicate and tricalcium aluminate). Understanding biomineralization at the nanoscale will help in the design of such materials as artificial bone and biocompatible ceramics.
Understanding how molecules dissociate or break apart is a crucial part of chemistry. Most molecules fall apart one step at a time. But some can break apart in concerted fashion, as happens in "three-body dissociation." Analyzing how three chemical bonds break simultaneously is a major challenge, because electronic states and degrees of freedom are numerous and complex. With a supercomputer at the University of Southern California’s Center for High Performance Computing and Communications, a team led by Anna I. Krylov and Vadim Mozhaevsky calculated energies for an extremely large number of possible atomic configurations of a molecule called sym-Triazine; its chemical structure, similar to benzene, has threefold symmetry. The molecule allows study of electron capture dissociation, an important process occurring naturally in interstellar space and the upper atmosphere, and used in laboratories to determine sequences in small proteins. When Krylov’s team represented the energies as a multi-dimensional plot called a potential energy surface, it turned out to bear a haunting resemblance to a flower. Each "petal" and "leaf" is a two-dimensional slice of one of the many electronic states of sym-Triazine; the spectrum of colors represents the energy of those states.