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CASC AT 25: CELEBRATING A MILESTONE IN COMPUTING EXCELLENCE

The year was 1990. Engineers were preparing the Hubble Space Telescope for launch. A hot new handheld video game, the Nintendo Game Boy, was flying off the shelves. The Human Genome Project was in its infancy. By year’s end, there was but a single website on what would become the World Wide Web.

It all sounds quaint now, but it was the cusp of a new era. From certain vantage points, it was possible to see glimpses of the incredible transformations that computers would soon bring to the world. Supercomputers were proliferating at universities and other research institutions around the country, crunching data at an unprecedented pace and yielding thrilling new discoveries in physics, engineering, and astronomy. The networks developed to link U.S. supercomputer centers, NSFNET and ESnet, were maturing into a major part of the Internet’s backbone. The High Performance Computing Act, spearheaded by then-Senator Al Gore, delivered the funds that would ultimately build the “Information superhighway,” deliver the first Web browser, and pave the way for the massive technology-driven commercial, scientific, and cultural shifts to come.

Against this backdrop, the Coalition for Academic Scientific Computation (CASC) was born. The leaders of university supercomputer centers faced increasing challenges as the demand for high-performance computing resources ballooned, but people with relevant expertise and experience were few and far between. Finding no other organization with the expertise they needed, they started their own.

“The supercomputing center directors had no place to come for information and collaboration that was specifically for them,” reflects Sue Fratkin, CASC Washington Liaison. “That’s why CASC was created, and why it has lasted and grown. There’s no other place where these folks can come together and focus on their shared issues, problems, and solutions.”

From 12 founding members in 1990, CASC has expanded to 79 organizations across the nation, a growth that reflects not only the increased prevalence of high-performance computing, but also the value of bringing together the nation’s high-performance computing experts to exchange ideas, solve problems, and envision the future.

The Early Days: Tech’s Roaring ’90s

The 1990s were heady times for scientific computing. Year after year, the promise and potential of high-performance computing spread like wildfire into new fields, expanding from physics and astronomy to chemistry and then to biology. Today nearly all academic domains, as well as medical schools and hospitals, routinely tap supercomputer resources. Researchers supported by the Department of Energy, NASA and other federal agencies are also leaders in scientific computing.

“In the ‘80s, there were just a few fields that knew the value of high-performance computing and knew how to use it,” recalls Jim Bottum, Vice Provost and CIO for Computing and Information Technology at Clemson University. “Today, 88 percent of the academic departments at Clemson are using it.”

No longer confined to only the most elite universities and national laboratories, supercomputer centers began springing up all across the country. In parallel with this increasing availability of supercomputers—and typical desktop computers, for that matter—was the growth and widespread adoption of the Internet. As the enormous potential of the digital economy grew more apparent, businesses soon followed in the footsteps of academia, investing in their own high-performance computing resources. The decommissioning of NSFNET in 1995 marked a significant transformation: the network and protocols developed by academia for research and education were unleashed to the world at large, providing a vast new platform for countless commercial endeavors and fueling a cultural transition that pervades daily life today.

From the Fringes to the Mainstream

The tech boom of the 1990s led to unprecedented advances in how science was done. Ever faster processors, ever larger storage capacity, and ever more sensitive instrumentation rapidly expanded the capacity to harvest data from our world and carry out the analyses to make sense of it. To take advantage of these new technologies, the supercomputing world underwent a monumental transformation, moving from vector machines to the massively parallel systems that are now taken for granted. Computing grew ever more central to scientific discovery, spawning fields like computational chemistry and computational biology.

All of this happened so quickly that now, even those terms are outdated. “The phrase ‘computational science’ has become redundant, as it is impossible to conduct scientific research without using computational methods,” says Dan Reed, Vice President for Research and Economic Development at the University of Iowa.

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BREAKING HIGH-TECH MATERIALS VIRTUALLY
(SO IT DOESN'T HAVE TO HAPPEN IN REAL LIFE)

Ceramic matrix composites are known for withstanding incredible heat and pressure—that’s why they’re used everywhere from spaceship heat shields to car brakes. In the hunt for ever more durable materials, Hrishi Bale and Rob Ritchie at Lawrence Berkeley National Laboratory are using information from state-of-the-art X-ray micro-tomography techniques to enable computer simulations to predict how and when these materials might fail. They’re also combining laboratory tests with computation to analyze how cracks propagate when new materials are subjected to extreme conditions. This 3-D rendering shows the miniscule breaks in the fiber of a ceramic matrix composite that has been heated to 1,750° Celsius. The visualization was made possible by crunching huge amounts of data generated when the test material was scanned with a powerful X-ray scattering technique to provide the 3-D real-time feedback necessary to accurately model failure in a virtual system. Understanding how materials fail in the laboratory can help prevent catastrophic failures in real life.

ULTIMATELY, THE CREATION OF NEW MATERIALS BOILS DOWN TO MIXING AND MATCHING THE INGREDIENTS WE HAVE ON HAND—the elements in the periodic table. Boris Yakobson and colleagues at Rice University in Houston, Texas developed a new theoretical framework to predict what will happen when certain combinations of elements are mixed together. The calculations were carried out on systems of the National Science Foundation’s Extreme Science and Engineering Discovery Environment (XSEDE) and on Rice University’s DAVinCI supercomputer cluster. The results are illustrated in this image, which shows the flower-like symmetry of the alloys intermingling with the cells of the periodic table. This work provides useful guidance for engineers seeking to design new materials for transistors, solar cells, and other applications.
GOING NANO: BIG INNOVATIONS AT SMALL SCALES

For the next big breakthroughs, scientists are thinking small—really small. Nanotechnology offers enormous new opportunities for innovation in materials science, electronics, medicine, and more. Computational resources are critical to advancing this burgeoning field.

Carbon nanotubes are tiny cylinders prized for their unique ability to conduct heat and electricity. Typically, they grow as a random assortment of tubes with various properties; scientists must then sort through them to find the tubes with the right mix of properties for specific applications. At Rice University, researchers are turning that process on its head by modeling the formation of more than 4,500 different carbon nanotubes to determine how to control the electrical properties of these tubes from the start, as they grow from the caps down. This image conceptually illustrates the relationships between end-cap shape and electrical properties for a subset of the 4,500 configurations studied. Calculations were carried out using resources that are part of the NSF’s Extreme Science and Engineering Discovery Environment (XSEDE) and on Rice University’s DAVinCI supercomputing cluster.

LEDs offer great potential for high-efficiency lighting. But engineers still grapple with what's known as the ‘green gap,’ a portion of the light spectrum where the efficiency of LEDs plunges. Using the supercomputing facilities of the Lawrence Berkeley National Laboratory, researchers at the University of Michigan, Ann Arbor are tapping into nanotech to develop more efficient LEDs. The researchers discovered that the semiconductor indium nitride, which typically emits infrared light, will emit green light if reduced to 1 nanometer-wide wires. Moreover, just by varying their sizes, these nanostructures could be tailored to emit different colors of light, which could lead to more natural-looking white lighting while avoiding some of the efficiency loss today’s LEDs experience at high power.

At the University of Texas at Austin, researchers are applying nanotechnology to develop new uses for molybdenum disulphide, a compound used as a lubricant and in petroleum refining. This image shows a close-up view of multilayered molybdenum disulphide stacked in a diamond anvil cell. Running electric leads through the structure, researchers can trigger electronic transitions and manipulate the mechanical, electrical, and optical properties of this innovative layered nanomaterial.
For 30 years, Elizabeth Davis endured painful and debilitating leg spasms daily, forcing her to rely on crutches and eventually confining her to a wheelchair. None of her doctors could figure out why. Then she enrolled in NCGENES, a project that sequences the genomes of patients with undiagnosed conditions in the hope of pinpointing possible genetic causes. The project revealed Davis had dopa-responsive dystonia, a problem with the nervous system caused by a genetic mutation. The condition is easily treatable with medication, and less than two months after her diagnosis, Davis was able to shed her wheelchair and crutches and now walks on her own.

Davis’ remarkable story illustrates the impact that genomic analysis can have on ordinary people. The NCGENES project, led by Jim Evans at the University of North Carolina at Chapel Hill with analysis and data management support from the Renaissance Computing Institute (RENCI), advances genomic science through an innovative cyberinfrastructure and streamlined analysis process that helps researchers and doctors work together to find genetic abnormalities, make diagnoses, and when possible, find treatments. So far, about 750 patients have enrolled.

Researchers at the pharmaceutical research firm Janssen Research & Development were stymied. Why were some rheumatoid arthritis patients responding well to a new therapy, while others were not? They had an inkling that the patients’ genes might provide a clue, so they obtained genetic samples from 438 patients. But performing the necessary analysis would have taken a regular computer about four years working 24/7. It was too long to wait.

The research team turned to the San Diego Supercomputer Center at the University of California, San Diego and the Scripps Translational Science Institute for help processing the massive data sets. The bulk of the analysis was completed in six weeks, allowing researchers to move forward with refining the new arthritis therapy.

The enormous time savings was achieved thanks to the thousands of cores available on the Gordon supercomputer (shown in the image) and its innovative use of flash memory – the kind that’s used on a typical USB thumb drive, only on a huge scale. Starting with 50 terabytes of data from patients’ DNA, developers used open source software tools to construct a 14-step processing pipeline and creative solutions to store and manage the data. The collaboration demonstrates the growing need for large-scale, high-performance computing resources to turn raw genetic data into results that can inform treatment and drug discovery.

Incredibly, some sea creatures, such as comb jellies, can fully regenerate their brains and nerves when injured. It’s a tantalizing prospect for scientists looking for ways to help people who suffer catastrophic brain or spinal cord injuries. The problem is that studying these amazing sea creatures is difficult because their bodies begin to disintegrate and their genetic make-up begins to change within minutes after being hauled to the surface. Enter researcher Leonid Moroz and the University of Florida’s cutting-edge floating genomic laboratory on the super-yacht Copasetic. The ship allows scientists to take samples from the sea anywhere in the world, immediately process them for genetic analysis, beam the raw data to the UF supercomputer HiPerGator, and receive the results back within hours. The arrangement offers a highly efficient way to scour the seas for new medical insights.
ENGINEERING ANTIDOTES

Though they are perhaps best known for their use in weapons, organophosphorus chemical nerve agents are also found in some industrial and household pesticides. These products can be just as deadly as weapons when people are purposefully or accidentally exposed to them. In the quest for new fast-acting nerve agent antidotes, researchers at the Ohio State University are using sophisticated methods to harness the body’s own natural defenses. Modeling the chemical structure of modified human enzymes on the powerful parallel supercomputer systems at the Ohio Supercomputer Center has put the researchers on a promising path to developing a single enzyme capable of deactivating many different nerve agents. The project is part of a collaboration between Ohio State University, the U.S. Army Medical Research Institute of Chemical Defense, and Israel’s Weizmann Institute of Science.

DECODING BREAST CANCER

Innovative visualizations like these, powered by data-crunching at a massive scale, are helping researchers parse emerging data on breast cancer causes and cures.

(Top) University of Pittsburgh researcher Ryan Hartmaier developed this map of the genomic variations that are acquired during the progression of metastatic breast cancer. The outer ring represents the chromosomes of the human genome. The next two circles show point mutations—single letter changes in the DNA sequence—acquired in metastatic breast cancer. The arcs in the center represent structural changes (when a part of the genome is moved from one place to another). These structural changes are technically and computationally difficult to identify and require advanced genome alignment algorithms that consume vast computational resources. Processing the data necessary to produce these complex wheels for each of 20 patients took 144 computer processors more than 157,000 CPU hours.

(Bottom) This image, from researchers at Rice University, shows changes in the levels of key proteins in cancer cells during four different treatments. Each wedge represents a protein, broken into four sub-sections representing the four treatments. Each concentric ring represents a time point at which the protein level was measured. The blue linkages in the center identify suspected interactions among the proteins. The goal of the research is to improve cancer treatments by illuminating precisely how different treatments affect cancer cells.

HOMING IN ON ALZHEIMER’S

Despite the increasing prevalence of Alzheimer’s disease, its precise causes—and effective treatments—remain elusive. Researchers are now applying the power of supercomputing to trace the origins of the amyloid oligomers that form in the brains of Alzheimer’s patients. These images represent some of the possible ring-shaped oligomers that can form from selected configurations of amyloid-beta peptides on the membranes of brain cells. San Diego Supercomputer Center researcher Igor Tsigelny surveyed the possible dynamics of these peptides and their interactions to predict how they might organize into oligomers that would be able to penetrate the membranes and eventually lead to cell death. Although the results are theoretical, they give researchers clues about how to identify real-world problem proteins and peptides and could lead to new targets for drug development.
CAN WE BURY OUR CARBON PROBLEM?

Carbon sequestration has been proposed as a way to reduce greenhouse gas emissions and curb climate change by injecting carbon dioxide deep underground. But figuring out how to do it properly—and whether it would even work—takes sophisticated modeling. This colorful model, produced by David Trebotich and the Energy Frontier Research Center for Nanoscale Control of Geologic CO2 at Lawrence Berkeley National Laboratory, simulates the chemical interactions between CO2 and deep rock formations to help predict whether sequestered carbon would stay buried or seep up through tiny fissures.

Crunching billions of data points, the model shows pH variations across grains of the mineral calcite at a resolution of one micron (one-millionth of a meter), making it the first to examine reactive transport processes associated with carbon sequestration at such a fine level of detail. Ultimately, this fine-grained model can be merged with large-scale simulations to inform smart engineering solutions. Trebotich is applying similar simulation techniques for insights on hydraulic fracturing and other energy applications.

SPACE WEATHER AND THE WORLD’S ELECTRIC GRID

As we become ever more dependent on the marvels of modern electricity, we also become more vulnerable to the effects of space weather—highly charged particles from the sun that could potentially bring down large swaths of the world’s electric grid, disrupt communications networks, and damage electronic devices. These particles are pushed into space from strong magnetic storms on the surface of the sun; they then race across 93 million miles and pummel the Earth. Although Earth’s own magnetic fields shield us from most of these particles, some can get through if the storm is strong enough. In the past, space weather has caused localized blackouts lasting hours; larger storms in the future could have much worse effects.

To get a better handle on the threat posed by solar storms, researchers at the University of California, San Diego and Lawrence Berkeley National Laboratory have teamed up to develop this remarkable visualization of the tumultuous magnetic field in the solar wind. Produced with supercomputers at the National Institute of Computational Sciences, it is the first simulation to cover the details of the magnetic field for such a wide range of scales at once—from planet-sized phenomena to subatomic dynamics—making it the most detailed representation of solar wind to date.

STAR POWER

Plasma—which makes up the sun and other stars and is the most abundant form of matter in the universe—could hold the secret to new nuclear fusion technologies capable of providing vast amounts of usable energy. But to harness the power of plasma, we first must learn to control it in a laboratory setting.

In support of that quest, Wendell Horton and colleagues at the University of Texas at Austin developed these models of the plasma vortices that are formed by ionized gases in Earth’s upper atmosphere. These naturally-occurring plasma structures have been known to disrupt radio communications and GPS systems. The visualization traces the evolution from a coherent vortex to a disordered state; the research team is investigating the factors that lead to instability to support the ultimate goal of confining and controlling plasma for nuclear fusion.
CALCULATIONS FOR CLEANER AIR

Despite its reputation for outdoor adventures and pristine mountain wilderness, Utah is home to some of the country’s worst air pollution. The state’s mountainous geography traps noxious pollutants in its population centers—in particular, around the Salt Lake City area—for days or weeks at a time, shrouding more than a million residents in a blanket of smog. Studies have linked high levels of air pollution to increased rates of asthma, autism, heart disease, childhood cancers, and infant mortality.

In partnership with the University of Utah’s Center for High Performance Computing, the photochemical modeling group at the Utah Division of Air Quality developed high-resolution simulations to determine the effectiveness of fine particulate mitigation strategies and tailor an emissions program to incorporate the results. Advanced computing resources help the division’s air quality modelers accomplish the analyses in less than one-fifth the time it previously took, allowing a more responsive and flexible pollution response strategy.

CATALYZING ADVANCES IN SOLAR TECHNOLOGY

Transforming solar energy into a storable source of liquid fuel—"solar fuel"—requires researchers to become sophisticated chemical matchmakers. Like matchmaking in the human sphere, the act of promoting a desired chemical reaction (called catalysis) depends on an intricate understanding of how molecules behave under specific circumstances. Although researchers have developed powerful computer models to predict catalysis, these models have not traditionally accounted for relativistic effects, which derive from the theory of relativity and are most important for calculations involving the heavier elements of the periodic table. These elements also happen to show the greatest potential as catalysts for solar fuel cells.

To address this gap, researchers calculated the distribution of electrons in molecules containing Ruthenium, one element being investigated for applications in solar fuels, both with relativistic effects and without. One result, shown in this visualization, reinforces the need to incorporate relativistic effects into the computational model. The project, a collaboration between the Renaissance Computing Institute and the University of Texas at San Antonio, could also could have implications for catalysis models involved with nuclear waste, industrial chemicals, and materials design.
Visualization is a way to make the invisible visible

Donna Cox, director of the Advanced Scientific Visualization Laboratory at the National Center for Supercomputing Applications

Visualization—the translation of data into visual form—is a potent tool for scientific analysis. Without images and animations, much of the output from even our greatest supercomputers would be simply a jumble of numbers, obscuring the patterns locked within.

“Visualization is the highest-bandwidth path between computing and the brain,” says Wes Bethel, a senior computer scientist and head of the Visualization Group at Lawrence Berkeley National Laboratory. It is a pathway that often leads to insights that inform real-world decision making.

Our visualization capacity has advanced tremendously over the past quarter-century. Donna Cox, director of the Advanced Scientific Visualization Laboratory at the National Center for Supercomputing Applications wants to determine how a bacteria-infecting virus packages its DNA during a critical step in its life cycle, the available visualization tools just weren’t cutting it. So they invented a new technique, allowing the user to vary the visualization’s focus to clearly resolve how each component relates to its neighbors. The team found that the individual components do not always line up in the same way, as was previously thought. The visualization technique could have many other potential applications.

Necessity is the mother of invention may be cliché but it is an undeniable tenet of scientific visualization. When Wen Jiang and colleagues at Purdue University wanted to determine how a bacteria-infecting virus packages its DNA during a critical step in its life cycle, the available visualization tools just weren’t cutting it. So they invented a new technique, allowing the user to vary the visualization’s focus to clearly resolve how each component relates to its neighbors. The team found that the individual components do not always line up in the same way, as was previously thought. The visualization technique could have many other potential applications.
25 Years of Visualizing Incredible Discoveries

This is not a bubble. In fact, it is one of the most sophisticated computer-generated visualizations created to date. Developed in 2013 by Lawrence Berkeley National Laboratory mathematicians Robert Saye and James Sethian, the animated version of this strikingly realistic model shows how the bubbles’ surfaces quiver as they pop and reform into a smaller and smaller cluster. Along the way, their surfaces continue to reflect their (virtual) surrounding environment. Such computational feats have applications in both science and industry.

Created in 1994, this image is an early example of the extraordinary level of detail supercomputers have made available to biomedicine. This colorful visualization shows the electrostatic potential and electric field generated by an enzyme engineered from the intestinal bacterium E. coli, a bacterial species that can present serious health risks and has served as a model in biotechnology research for more than 60 years. Created by researcher Daniel Ripoll using the first massively parallel supercomputer system at the Cornell Theory Center (known today as the Cornell Center for Advanced Computing), the image yields important insights on the enzyme’s role and activity.

Laboratory at the National Center for Supercomputing Applications, recalls the groundbreaking simulations of thunderstorms that were developed in the early 1990s. At the time, it was incredible to be able to see an entire virtual storm, and the models shed new light on how storms form and dissipate.

Today, supercomputer-driven visualizations can tackle similar questions at a much greater level of detail. Today’s visualizations, for example, allow scientists to drill down from the huge scale of a storm system, which can stretch across several states, to the relatively miniscule scale of a tornado forming within the storm’s heart. Such investigations, in turn, lead to better weather prediction capabilities and more accurate early-warning systems.

“That example shows that it’s not just about pretty pictures,” says Cox. “Visualization is a way to make the invisible visible. It gives us the scientific insights necessary to understand the anatomy of these disasters in order to prevent them.”

Combining high-powered analytics with visualization can help researchers pick out features such as small tropical cyclones from global climate simulations, yielding greater insight into the effects of climate change.

Scientific visualization has evolved in parallel with the Hollywood graphics industry. “In the early 1990s, we began having meetings together to harness the tools of the industry and bring them into the world of science,” recalls Cox. “Then there was this incredible cross-pollination. Even today, there is a constant exchange—gaming interfaces, for example, are always stretching the boundaries of what we can accomplish.”

Thanks in part to industry-academia collaborations, the human-computer interface has improved dramatically, allowing scientists and decision makers to interact with visualizations, manipulating variables on the fly to get results in real-time. An ongoing collaboration between Argonne National Laboratory and NCSA, for example, has produced an interactive visualization of real-time traffic patterns to help manage evacuations during disasters.

“Advances in visualization have added to our productivity and innovation in this country,” says Cox. “But not only does visualization have the power to bring scientific insight, it also has tremendous power to educate the public about why science is relevant to their lives.”
Adapting to Our Changing Planet

STORM CHASERS
Improved forecasting and early warning systems have dropped the death toll of tornadoes significantly over the past few decades. But they remain a very real threat to lives and property, especially across the swath of the south-central United States known as “Tornado Alley.” Researchers at the University of Oklahoma and the University of Texas at Austin have developed highly-detailed simulations that reveal the complex inner workings of thunderstorms in order to better predict when tornadoes will emerge.

Shown here is a simulated storm that has spawned a tornado. The scene illustrates how a vortex ring forms when a strong updraft punches into the stable stratosphere, causing the surrounding air to curl downward. Such simulations give researchers insights on the conditions that are likely to herald the development of a tornado.

MAPPING VANISHING FORESTS
Changes in forest cover have major environmental and economic implications. For example, forests play a key role in mitigating climate change by absorbing carbon. This map—the first-ever high-resolution global map of forest extent, loss and gain—was created by a multi-disciplinary team led by Matt Hansen at the University of Maryland that included researchers from universities, Google, and government agencies. The analysis shows a global loss of 888,000 square miles of forest and a gain of 309,000 square miles of new forest between 2000 and 2012. Colors indicate forest loss (red), gain (blue), and a mix of loss and gain (purple/magenta). Density of tree cover is indicated on a scale from 0% (black) to more than 80% (green). Drawing data from more than 650,000 images collected by the Landsat satellite, the analysis is the first map of forest changes at a level of detail that is both locally relevant and globally consistent.
WEATHER WIZARDRY

High-performance computing allows researchers to analyze weather phenomena at a greater level of detail than has ever before been possible, strengthening our forecasting abilities and enabling more effective response strategies.

(Left) Lake-effect snow, produced when cold winter winds move across warm lake water, brings joy to skiers and headaches to commuters. Despite dramatic forecasting advances over the past few decades, the lake effect remains difficult to predict. University of Utah researcher Jim Steenburgh and colleagues are integrating field data with computer models to pinpoint the environmental conditions that produce lake-effect precipitation, allowing local officials and residents to more effectively anticipate and respond to these weather events.

(Right) This graph provides a detailed model of the lowest part of the atmosphere across 36 square kilometers of land. The colors indicate variations in the “potential temperature”—that is, the temperature that would occur in the absence of cooling or warming effects caused by the vertical relocation of air. Because the simulation accounts for turbulence in the atmosphere, it offers a much more detailed view of the atmosphere’s structure than is possible with current weather models that have much coarser resolution. The model was developed by Song-Lak Kang of Texas Tech University.

ANIMAL TRACKS

To protect threatened species, we need to better understand them. Researchers have long attempted to trace the habits of animals by tagging them and following their movements, but the vast amount of data that can now be streamed with such approaches often leaves researchers scrambling just to keep up with the deluge of data. Scientists from the U.S. Geological Survey and the San Diego Zoo’s Institute for Conservation Research teamed up with the San Diego Supercomputer Center to develop a tracking method that combines 3-D and advanced range estimator technologies to monitor the movements of three threatened species at an unprecedented level of detail: California condors, giant pandas, and dugongs (a marine mammal somewhat similar to the manatee). Thanks to the supercomputer resources, calculations that had formerly taken four days to complete can now be finished in less than half an hour, allowing the researchers to stay hot on the trail of these vulnerable species.
Few scientific questions are as fundamental, or fascinating, as the origin of the universe. Luckily, it is possible to see vestiges of the early universe by looking at the galaxies farthest away from us. Because it takes light from these galaxies about 13 billion years to reach us, our strongest telescopes capture the light that these galaxies created just a few hundred million years after the Big Bang—baby pictures, by cosmic standards. Scientists are combining these observations with computer models to reconstruct the early history of the universe.
BUBBLES AFTER THE BIG BANG

Only nanoseconds after the Big Bang, the universe began cooling and forming bubbles, which grew, collided and coalesced. Researchers Jim Mertens of Case Western Reserve University, and Tom Giblin of Kenyon College, study such processes in the infant universe in order to better understand how early matter behaved and eventually evolved into structures like stars and galaxies that we observe today. This simulation, created using supercomputing resources at Case Western Reserve, Kenyon, and the Ohio Supercomputer Center, examines the early evolution of such bubbles.

EYES ON THE SKY

Ever spent a pleasant summer evening gazing up at a moonless sky, trying to count the stars? The Sloan Digital Sky Survey (SDSS) does just that—and more—on a massive scale. Now entering its 15th year, the project is responsible for the most detailed 3-D maps of the universe ever made. Using this 2.5-meter telescope at Apache Point Observatory in New Mexico, the project systematically surveys the stars in the Milky Way Galaxy, the architecture of galaxies in the nearby universe, and the large-scale structure of the entire cosmos. Project researchers combine the incredible power of the telescope with sophisticated digital detector technology and intense computation to yield a steady flow of rich information about our universe. To effectively deal with the enormous amount of data it generates, the SDSS partners with the University of Utah’s Center for High Performance Computing to deliver an integrated system for storage, algorithm development, pipeline processing, and worldwide distribution of astronomical survey data.

HOW TO SAMPLE AN ASTEROID

Asteroids can yield important clues about our solar system and universe. Researchers believe it is possible to sample asteroids by shooting projectiles at them and then collecting the asteroid pieces that scatter from the site of impact. Derek Richardson and colleagues at the University of Maryland, College Park developed this simulation to help determine how projectile shape, speed, direction, and other factors would influence the quality of samples a space mission could collect using this method. The particles are represented as glass beads, which are color-coded to represent different starting layers within the asteroid.
Inspiring Tomorrow’s Innovators

MAKING SCIENCE ACCESSIBLE
For people with disabilities, working in a typical wet laboratory can be a daily exercise in frustration. From sinks and fume hoods that can’t accommodate a wheelchair to safety showers and eye wash stations that are just out of reach, the physical constraints of working in a lab can inadvertently turn bright and motivated students away from careers in science. Purdue University engineers and researchers took this problem by the horns when they developed the Accessible Biomedical Immersion Laboratory, a biology wet lab designed with accessibility in mind. The lab has such features as a powered adjustable-height lab bench, a talking scale, and a motion-activated biohazard disposal bin.

A new 3-D virtual version of the real-world lab brings the team’s innovative accessibility solutions to the world. Using a variety of immersive 3-D display environments, users can navigate the virtual model to explore the lab’s accessibility features from standing height or from the perspective of someone sitting in a wheelchair. Purdue’s hope is that the virtual model will help labs around the world better accommodate people with disabilities to make science accessible to all.

MOTIVATING GIRLS TO GEEK OUT
Software jobs now outnumber qualified applicants three-to-one, yet 90% of U.S. high schools still do not teach computer science. What’s more, girls are far less likely than boys to take advantage of computer science opportunities at the high school and college levels, contributing to a cycle of underrepresentation of women in the computer science workforce (as well as STEM fields more broadly).

To address these gender and workforce gaps, the San Diego Supercomputer Center, in partnership with local universities and industry support groups, recently launched GirlITech San Diego, a non-profit program aimed at encouraging young women to learn and apply computing skills. The program supports after-school computing clubs targeted toward girls and women from the middle school to the undergraduate level.
**VISUALIZING DIVERSITY (IN VISUALIZATION)**

Visualization—visually representing raw data to glean insight and understanding of the complex relationships hidden within—is a growing field with an incredibly diverse array of career opportunities, ranging from hard science to Hollywood. However, women and minorities have consistently been underrepresented in visualization careers and training programs. The Computer Research Association’s Committee on the Status of Women in Computing Research and the Coalition to Diversity Computing (CRA-W/CDC) Broadening Participation in Visualization Workshop, hosted by Clemson University in 2014 and organized by Vetria Byrd, Clemson’s Director of Advanced Visualization, was the first workshop designed to broaden participation in visualization by focusing on the participation of women and members of underrepresented groups. Providing ample opportunities for networking and mentoring, the workshop was designed to inform, inspire, and encourage participation of individuals from diverse backgrounds to consider visualization as a career path.

Past meets future in this unique interactive visualization of Kentucky’s Mammoth Cave. Designed to broaden access to the geosciences, the simulation serves as a virtual field trip to give students with disabilities a chance to explore cave formations they couldn’t otherwise access. In addition to learning geoscience principles, students get a taste of the region’s cultural history through a tour guide avatar modeled on Materson Mat Bransford, a real-world slave who led tours of the cave in the early-to-mid 1800s. The simulation was created by a team of students and researchers who collected high-precision data from the cave using laser remote-sensing technology and high-resolution digital photography, gathered historical data to create an authentic tour-guide avatar, and integrated the data into a virtual environment. The project is a collaboration of the Ohio Supercomputer Center, Georgia State University, Ohio State University, and several non-profit research and education organizations and is funded by the National Science Foundation OEDG Award 1108127.

**SPARKING NEW INSIGHTS BY BRINGING THE PAST TO LIFE**

Wandering through a simulated cave or an ancient Roman temple may sound like a video game, but these innovative creations go beyond mere entertainment. 3-D computer models are increasingly being used not just to depict imagined worlds, but to reconstruct actual human history. Two student-led projects advance understanding of days past—while simultaneously equipping a new generation to take interactive visualization to the next level.

This interactive depiction of a Roman temple was created by a group of Rice University students studying archaeology, anthropology, art history, architecture, and engineering. Shown here on Rice’s DAvinCI Visualization Wall and available to scholars online, the model lets users walk through the virtual temple and learn about its architectural and aesthetic features. Students created a similar model of a 15th-century Swahili residence based on field data gathered by archaeology students during a summer dig. Constructing the models required creative thinking as students tackled knowledge gaps that scholars had not previously solved and raised new questions in the process.
Technology advanced in leaps and bounds through the early 2000s and 2010s, allowing scientists to complete the human genome project years ahead of schedule. GPS proliferated throughout the sciences and daily life. Satellites beamed enormous quantities of data down to Earth, yielding new insights on everything from outer space to city planning. The era of what is now called “Big Data” began.

Once confined to the fringes, high-performance computing grew to pervade not only science, but society. “Today, high-end computing is, in a sense, ubiquitous. A smart phone is now more powerful than the systems that NASA used to put men on the moon,” says Fratkin.

Looking back over CASC’s history, Reed says things have come a long way not just in terms of technical advances and computing applications, but in people’s perceptions of the field: “Computing writ large has penetrated the popular culture in unprecedented ways. People are much more aware of the effects of computing and technology than they were 25 years ago. Information technology is recognized as a valued career, as a contributor to global interaction, and as an enabler of innovation and discovery.”

As 2015 begins, it is all too easy to see the tremendous advances of the past 25 years as somehow preordained. But the truth is, each step—each technological advance that led to the next and then the next—required an enormous amount of expertise and strategic research investment. That investment must not stop now, especially not in research computing, a sector that has for decades served as the start of the pipeline fueling business innovation and economic growth.

“If you’re going to be a major research university, you must have a high-end computing center because there’s no way that your faculty can do the research without this resource,” says Fratkin. “But although this technology is as ubiquitous as the telephone, it’s not the telephone. There are far greater investments that must be made.”

Those investments have become increasingly critical as computer scientists grapple with new physical constraints. “We’ve been conditioned to believe that computers will get ever faster and ever cheaper, and to assume supercomputers will do the same,” says Reed. “The end of Dennard scaling [which until recently has allowed us to develop smaller, faster chips at an ever lower price] has profound implications for our future. What we do next in terms of research investment will shape our future. We need new approaches to scalable software, energy management, reliability and resilience, and processor architecture and technology.”

America’s innovation pipeline depends on universities and national laboratories staying at the cutting edge, says Fratkin. “High-end computing at universities is central to states’ economic development, but states aren’t putting in the level of investment that’s needed.” Founded during a time of great national investment, CASC has recently had to shift its focus to addressing the waning budgets of its member organizations. “Right now is the toughest time for the CASC membership in terms of sustainability of their programs,” says Fratkin.

Even for smaller universities, computing resources are critical to the type of research activities that will maintain America’s role as a leader in global science and technology, says Clemson’s Jim Bottum. “It is remarkable that even in our fad-obsessed world, computing resources remain as critical today as they were in the 1980s and 1990s, if not more so. With big data, the challenges are just getting bigger, and the nation needs to invest in computational resources now more than ever.”
CASC Membership

Arizona State University
Advanced Computing Center
Tempe, Arizona

Boston University
Center for Computational Science
Boston, Massachusetts

Brown University
Center for Computation and Visualization
Providence, Rhode Island

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

Carnegie-Mellon University & University of Pittsburgh
Pittsburgh Supercomputing Center
Pittsburgh, Pennsylvania

Case Western Reserve University
Core Facility Advanced Research Computing
Cleveland, Ohio

City University of New York
High Performance Computing Center
Staten Island, New York

Clemson University
Computing and Information Technology (CCIT)
Clemson, South Carolina

Columbia University
Shared Research Computing Facility
New York, New York

Cornell University
Center for Advanced Computing
Ithaca, New York

Florida State University
Research Computing Center
Tallahassee, Florida

Georgia Institute of Technology
Atlanta, Georgia

Harvard University
Cambridge, Massachusetts

Icahn School of Medicine at Mt. Sinai
New York, New York

Indiana University
Bloomington, Indiana

Johns Hopkins University
Baltimore, Maryland

Lawrence Berkeley National Laboratory
Berkeley, California

Louisiana State University Center for Computation & Technology (CCT)
Baton Rouge, Louisiana

Michigan State University
High Performance Computing Center
East Lansing, Michigan

Mississippi State University
High Performance Computing Collaboratory (HPC2)
Mississippi State, Mississippi

National Center for Atmospheric Research (NCAR)
Boulder, Colorado

New York University
New York, New York

North Dakota State University
Center for Computationally Assisted Science & Technology
Fargo, North Dakota

Northwestern University
Evanston, Illinois

Oak Ridge National Laboratory (ORNL) Center for Computational Sciences
Oak Ridge, Tennessee

Princeton University
Princeton, New Jersey

Purdue University
West Lafayette, Indiana

Rensselaer Polytechnic Institute
Troy, New York

Rice University
Ken Kennedy Institute for Information Technology (K2I)
Houston, Texas

Rutgers University
Discovery Informatics Institute (DII2)
Piscataway, New Jersey

Stanford University
Stanford, California

Stony Brook University
Stony Brook, New York

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

Texas Tech University
High Performance Computing Center
Lubbock, Texas

The George Washington University
Institute for Massively Parallel Applications
Washington DC

The Ohio State University
Ohio Supercomputer Center (OSC)
Columbus, Ohio

The Pennsylvania State University
University Park, Pennsylvania

The University of Texas at Austin
Texas Advanced Computing Center (TACC)
Austin, Texas

University of Alaska Fairbanks
Arctic Region Supercomputing Center (ARSC)
Fairbanks, Alaska

University of Arizona
Tucson, Arizona

University of Arkansas
High Performance Computing Center
Fayetteville, Arkansas

University at Buffalo, State University of New York
Center for Computational Research
Buffalo, New York

University of California, Berkeley
Berkeley, California

University of California, Los Angeles
Institute for Digital Research and Education
Los Angeles, California

University of California, San Diego
San Diego Supercomputer Center (SDSC)
San Diego, California

University of Chicago & Argonne
National Laboratory Computation Institute
Chicago, Illinois

University of Colorado Boulder
Boulder, Colorado

University of Connecticut
Storrs, Connecticut

University of Florida
Gainesville, Florida

University of Georgia
Advanced Computing Resource Center (GACRC)
Athens, Georgia

University of Hawaii
Honolulu, Hawaii

University of Houston Center for Advanced Computing and Data Systems
Houston, Texas

University of Illinois at Urbana-Champaign
National Center for Supercomputing Applications (NCSA)
Champaign, Illinois

University of Iowa
Iowa City, Iowa

University of Kentucky
Center for Computational Sciences
Lexington, Kentucky

University of Louisville
Louisville, Kentucky

University of Maryland
College Park, Maryland

University of Michigan
Ann Arbor, Michigan

University of Nebraska
Holland Computing Center
Omaha, Nebraska

University of Nevada, Las Vegas
National Supercomputing Center for Energy and the Environment (NSCCEE)
Las Vegas, Nevada

University of New Mexico
Center for Advanced Research Computing
Albuquerque, New Mexico

University of North Carolina at Chapel Hill
Chapel Hill, North Carolina

University of North Carolina at Chapel Hill Renaissance Computing Institute (RENCI)
Chapel Hill, North Carolina

University of Notre Dame
Center for Research Computing
Notre Dame, Indiana

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

University of Pittsburgh
Center for Simulation and Modeling
Pittsburgh, Pennsylvania

University of South Florida
Research Computing
Tampa, Florida

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

University of Tennessee
National Institute for Computational Sciences (NICS)
Knoxville, Tennessee

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

University of Virginia
Alliance for Computational Science and Engineering
Charlottesville, Virginia

University of Washington
Seattle, Washington

University of Wisconsin-Madison
Madison, Wisconsin

University of Wisconsin, Milwaukee
Milwaukee, Wisconsin

University of Wyoming
Advanced Research Computing Center (ARCC)
Laramie, Wyoming

Virginia Tech University
Advanced Research Computing
Blacksburg, Virginia

West Virginia University
Morgantown, West Virginia

Yale University
New Haven, Connecticut