ONE STEP AHEAD
Fighting Emerging Threats and Fostering Innovation with Computational Science
Researchers at Purdue University mapped the structure of the Zika virus using advanced cryo-electron microscopy and high performance computers. Understanding the structure of the virus is a key step toward finding drugs or vaccines to stop this global disease threat. See page 4 for more details.
About CASC

The Coalition for Academic Scientific Computation is an educational nonprofit 501(c)(3) organization with 84 member institutions representing many of the nation's most forward-thinking universities and computing centers. CASC is dedicated to advocating for the use of the most advanced computing technology to accelerate scientific discovery for national competitiveness, global security, and economic success, as well as develop a diverse and well-prepared 21st century workforce. In addition, CASC collaborates with the United Kingdom High Performance Computing Special Interest Group (HPC-SIG) to advance the use of scientific computing across all disciplines, and to support economic and workforce development in high performance computing-related fields.
WHEN A FRIGHTENING DISEASE THREAT bursts onto the scene the way the Zika virus did in 2015, it is crucial to respond quickly. As the virus spread rapidly throughout Latin America, evidence began to accumulate linking the typically mild virus with significant birth defects in babies whose mothers had been infected while pregnant.

Around the world, public health researchers scrambled to learn as much as possible about the virus, including how it might be stunting the brains of developing infants, and to figure out how to stop it. Although Zika wasn’t exactly a new virus, it hadn’t been studied much before its emergence in the Western hemisphere, and the connection with birth defects raised the research to a new level of urgency.

Fortunately, scientists weren’t starting from scratch. Zika is a flavivirus, making it a cousin of dengue, West Nile, yellow fever and other well-studied diseases. Flavivirus experts leapt into action, isolating Zika from patients’ blood samples to investigate what the virus shares in common with its relatives—and what makes it different.

To understand Zika well enough to find its weaknesses, scientists needed to know the virus’s structure. In a matter of months from the start of the outbreak, researchers at Purdue University combined two cutting-edge technologies to create a detailed map of the virus. The first was cryo-electron microscopy, a technique that allowed researchers to obtain, from a very small viral sample, thousands of high-resolution images of the virus. The second was high performance computing, which provided the computing capacity necessary to stitch all of those images together into a cohesive computer model of Zika’s structure.

Michael Rossmann, PhD, Hanley Distinguished Professor of Biological Sciences at Purdue, and collaborator Richard Kuhn, PhD, Purdue Professor of Biological Sciences, led that research effort with support from post-doctoral researchers and graduate students in both laboratories. Over the course of a remarkable career spanning 60 years, Rossmann has tackled a large array of viral threats with innovative research, pushing the boundaries of virology and technology at every step. We asked him to describe his recent Zika breakthrough and reflect on what high performance computation has brought to the field.
Why is it useful to know a virus’s structure?

Rossmann: I’ll give you an analogy. If you knew nothing about cars and wanted to figure out how to make them stop working, the first thing you would do is open the hood and take the car apart to try to figure out how the parts make the car work. If you can do that, you can also figure out how to stop the car from working. So a virus is akin to this car, which we are trying to understand. By opening the hood, looking at it carefully, and taking it apart, we can try to stop it from working.

What role did high performance computing play in your work with Zika?

Rossmann: With electron microscopy, we get projections of the virus in different orientations. As an architect uses 2-D blueprints to create a 3-D view of a house, we can create a 3-D image of the virus by combining these projections. To obtain enough detail, you have to see the virus in many different orientations—tens of thousands of projections. Then you can use a computational process to find the relative orientation of each one and put them all together into the 3-D structure of the virus. We use a lot of computing power for that.

Looking back over your career, how has the practice of science changed as computational capabilities have grown?

Rossmann: There’s been an incredible turnaround in how we do things in the last few years. There are now many computer programs to do the work of finding the orientations of these particles and putting them together to reconstruct a 3-D structure from 2-D projections. The computational capability is absolutely crucial.

One of the viruses we work on is a common cold virus that exacerbates asthma. It’s a very difficult virus to produce in the laboratory. We obtained about a half a milligram of it from our collaborators, and within about two weeks, one of the students in my lab was able to produce the structure of the virus. This would be impossible with the technologies we used in previous work. My lab produced the first structure of any common cold virus back in 1985, and it took us about six years. Now, we can do it in two weeks.

Would you like to share any hopes or expectations for the future of computational science?

Rossmann: Computing has always been essential, and even today we have difficulty finding storage space for all of our data or getting enough computing time.
High performance computing is not only a crucial part of the basic research needed to understand and fight infectious disease—it also opens vast new opportunities for improving public health. From tracking the spread of disease with Google search queries to collecting real-time vital statistics with mobile devices, today’s public health researchers and practitioners are increasingly tapping into Big Data.

An ongoing study at the University of Chicago, for example, researchers are using Facebook to help curtail the HIV epidemic on Chicago’s South Side. The social media platform offers a unique window into social networks used by the South Side population in which HIV is spreading most rapidly: African American men ages 16 to 29. The goal of the project is to identify the key people within this demographic whom public health officials can work with to disseminate potentially life-saving information about how to get the right medications to treat HIV or to avoid contracting the disease.

To increase use of effective HIV treatment and pre-exposure protections, the research team uses an old methodology with a new twist. Understanding how people are connected to each other has long been an important focus in public health. For example, it can be useful to know which people have the most social connections, which people might act as a bridge between different groups, and which people are socially isolated. For the Chicago study, the researchers used Facebook friend lists to map the social network in their target community. After recruiting volunteers, they were able to get data from about 300 people with roughly 1,000 friends each.

With thousands of potential relationships to map, the researchers turned to the University of Chicago’s Midway supercomputer to process the data. The team is developing custom analysis tools to pinpoint key individuals in the community and design public health interventions that can reach the greatest number of people most efficiently. If it works, the approach could not only reduce the spread of HIV on Chicago’s South Side, but also translate to other regions or other public health challenges.
Universities have long been hubs of technological innovation. It was, after all, a team of California academics who, in 1969, created a technique for computer-to-computer communication known as packet-switching that ultimately paved the way for the Internet. Take your smartphone and remove any component that has its roots in government-funded academic research—the camera, for instance, or the screen, the voice-recognition software, or the Wi-Fi connection. The phone you would be left with would not be very smart at all; it would really only be a phone.

It is business that put the smartphone in your pocket and the Internet in nearly every aspect of our lives, but it is basic academic research—powered by government investment, for the most part—that forms the knowledge foundation for our tech-hungry world.

At the Renaissance Computing Institute (RENCI) at the University of North Carolina at Chapel Hill, three initiatives show what can happen when universities act not only as knowledge creators but also as venues for productive, non-competitive exchange among researchers, businesses and government agencies. In these efforts and in numerous others around the country, academic centers are finding common ground to build solutions with impacts far beyond the university gates.

one

National Consortium for Data Science: This thought leadership forum brings together researchers and businesspeople who are grappling with how to develop and apply the emerging field of data science to benefit their work. With members including IBM, General Electric, Drexel University, North Carolina State University, the Environmental Protection Agency and RTI International, the consortium hosts regular conferences, offers data science courses and administers a seed grant program for faculty members conducting industry-informed research. The goal of the consortium is to help America take advantage of the ever-increasing flow of digital data in ways that result in new jobs and industries, new advances in healthcare, and transformative discoveries in science and competitive advantages for United States industry.

two

iRODS Consortium: The product of nearly 20 years and $25 million in grant-funded research, the data management software known as iRODS (short for Integrated Rule-Oriented Data System) is today used by thousands of businesses, research centers and government agencies to manage the large, complex data sets that are now central to doing business or conducting research. What’s more, developers have struck upon a business model that allows them to offer iRODS as a free, open-source product while ensuring the software’s sustainability through a consortium of paying members who receive hands-on support and an opportunity to influence future directions. What started with federal funding is now developing into a self-sustaining venture that helps institutions around the world harness the power of Big Data.

three

South Big Data Regional Innovation Hub: RENCI and the Georgia Institute of Technology co-lead this one-year-old effort funded in part by the National Science Foundation. The South Big Data Hub is one of four regional Big Data Hubs that aim to build innovative public-private partnerships to address regional challenges such as healthcare, habitat planning and coastal hazards using big data and data analytics. Each of the four Big Data Hubs engage businesses and research organizations in their region to develop common big data goals that would be impossible for individual members to achieve alone. In addition to community-driven governance structures, the Hubs are developing “spoke projects” based on regional priorities and partnerships.
WE LIVE IN AN AGE in which cyber threats are paramount. Hackers can take down power grids or grab the wheel of a car from a thousand miles away. Data breaches expose the personal and financial information of millions of people so routinely that they barely make the news. Hospitals, companies and even police departments pay out tens of thousands of dollars to retrieve data stolen in brazen “ransomware” attacks. Even data safeguarded by the U.S. Department of Homeland Security, the FBI and the IRS may not be as secure as we’d like it to be.

We now face adversaries who are backed by the governments of other nations or by vast, sophisticated organized crime networks in addition to the more run-of-the-mill hackers looking for a buck or seeking fame. And while today’s astoundingly fast and powerful computers enable incredible advances in science and consumer technology, they also provide the computing strength for criminals and spies to crack systems once thought secure.

As our lives and finances grow ever more dependent on our devices and IT infrastructure, we grow more vulnerable—both as individuals and as a nation—to theft, fraud and the disruption of crucial services.

These trends are all too familiar to Von Welch, director of Indiana University’s Center for Applied Cybersecurity Research (CACR), one of a growing number of academic centers positioning themselves on the front lines of the cybersecurity challenge. Home to the Center for Trustworthy Scientific Infrastructure, a National Science Foundation-designated Cybersecurity Center of Excellence, CACR advances research and education to address cybersecurity threats across academia, government and industry.

The challenge for such university centers is to keep up with threats that are both here to stay, and constantly evolving. “There doesn’t seem to be a technological silver bullet on the horizon that’s going to solve these problems,” said Welch. “It’s more of an ongoing process, like we might think of other risk management procedures such as the role of auditing in the field of finance.”

EDUCATING A NEW GENERATION

Just as there will always be a need for auditors and police officers, there will always be a need for cybersecurity expertise. Universities are working hard to create a workforce that’s up to the challenge.

“Cybersecurity is becoming a profession now for the first time,” said Welch. “We’re creating a more formalized workforce and educational opportunities and paths for people who want to pursue careers in this field.” One example is the CyberCorps® Scholarships for Service program, which awards...
grants through the NSF to support students studying cybersecurity in exchange for a period of government service after graduation.

Perhaps equally important are the informal ways in which cybersecurity is being integrated into the broader sphere of computer science education, and even into interdisciplinary work with fields such as business and law. Welch pointed to a new emphasis on the skills needed to build stronger products and systems from the get-go: “It’s a lot easier to build a house that’s up to code than to show up and put fires out every week. So by having better developed software and IT infrastructure that’s more secure to begin with, we’ll ultimately make our jobs in the [cybersecurity] field easier,” he said.

**BRIDGING SECTORS TO SOLVE SHARED PROBLEMS**

Beyond their educational role, universities occupy a uniquely valuable niche in the world of computer science. Although tech companies get a lot of the credit for flashy new hardware and software, often the seeds of these products can be traced to university research. It is academia, for example, that typically lays the theoretical foundation that makes possible the “disruptive” technologies that wind up in our homes, vehicles, farms and factories. In the same way, academia, driven by a need to build cutting-edge cybersecurity systems to protect cutting-edge computational infrastructure, pushes the envelope on cybersecurity techniques and technologies that ultimately find their way into commercial products. “Universities are the big engine for research in computer science and cybersecurity,” said Welch.

Universities also tend to be well connected with each other, enabling the rapid exchange of ideas. REN-ISAC, for example, which stands for Research and Education Networking Information Sharing and Analysis Center, facilitates exchange among research and higher education communities to report, study and respond to cybersecurity incidents. The organization originated at Indiana University and now has more than 500 member institutions.

Critically, universities facilitate the translation of foundational research into practical applications, helping to solve security problems that stymie research, government and commercial systems alike. “Research can tackle some of the problems that don’t have the economic incentives that private industry requires,” said Welch. In this way, universities are key to enabling breakthroughs in ‘tragedy of the commons’ situations where the challenge is too pervasive, or too complex, for one stakeholder to address alone.

One example of this is a project known as the Software Assurance Marketplace (SWAMP). A collaboration led by multiple research institutions with support from federal funding, SWAMP makes it easier for developers anywhere—including the tech industry—to ensure their products are up to the latest cybersecurity standards and practices. By bringing together multiple software assurance resources into one package, SWAMP creates a sort of Swiss Army knife of tools, techniques and information that would be difficult or expensive for individual developers to piece together on their own.

As our citizens, businesses and government continue to endure dangerous cyberattacks, it has become clear that these breaches are not some sort of fluke or temporary setback, but a new normal. Universities—through partnerships with industry and government—are a crucial force in creating a skilled workforce that gives us the means to fight back.
RACING FOR AN EDGE IN NASCAR

There is nothing run-of-the-mill about NASCAR racecars. They are highly engineered to drive up to 200 miles an hour on an oval track for hours at a time. In order to design a car that is both safe and competitive under those stomach-churning conditions, Eric Jacuzzi of NASCAR R&D partnered with TotalSim USA and the Ohio Supercomputer Center to create Computational Fluid Dynamics simulations that depict, in minute detail, how these cars will perform during races. The goal is to understand the aerodynamics of the cars and the factors that influence their performance, both when driving alone and in race conditions with other cars.

This work helps NASCAR R&D to design regulations that improve the racing excitement for NASCAR fans, who value close racing and lots of passing on the track—an exceedingly difficult feat when driving on an oval track at top speed. This image above shows a simulation of the forces at work when two NASCAR racecars are in a nose-to-tail drafting configuration.

CRASH-TEST SMARTIES

Computerized crash-test simulations are far more sophisticated than traditional crash-test dummies. These simulations can run many more crashes much more quickly than would be possible with real vehicles, and they provide detailed data on how the muscles, tissue and organs in a real human body will react during a high-speed impact.

This image, from a model used by researcher Ashley Weaver of Wake Forest University and the Virginia Tech-Wake Forest School of Biomedical Engineering and Sciences, shows what happens when a driver is in a more reclined position during a high-speed collision. The research revealed that existing restraint systems may not fully protect drivers in a reclined position, underscoring the need to design seat belts that can account for different sitting positions to reduce serious injuries in crashes. Computational simulations were run on the Blacklight Supercomputer at the Pittsburgh Supercomputing Center and the DEAC Cluster at Wake Forest University. Weaver also benefited from support from the Extreme Science and Engineering Discovery Environment (XSEDE).
ENGINEERING THE CAR OF THE FUTURE

At Mississippi State University’s Center for Advanced Vehicular Systems, researchers Matthew Doude and David Francis are applying high-tech modeling to break the mold on car design. Using computational models conducted at the school’s High Performance Computing Collaboratory, the team takes a simulated Subaru BRZ and tests multiple design alterations, optimizing each component virtually before trying them out in the physical world.

This approach has yielded profound design improvements that just might find their way into your driveway before long. For example, replacing the car’s standard drivetrain with a hybrid version that sends power to electric motors at the rear wheels enabled four times greater fuel efficiency and improved performance. The team also redesigned the car’s subframe (top right). The mass of the new subframe, made from strong-yet-lightweight magnesium, was reduced by 40 percent as compared to the stock steel subframe.

The concept car shown at top left was built to demonstrate the new subframe component along with a variety of other cutting-edge automotive technologies. It boasts excellent handling and performance, and can drive 100 miles on just one gallon of gas, making it less oil-dependent and far more environmentally friendly.

DESIGNS THAT TAKE FLIGHT

Although passengers know it best as the cause of the dreaded “Fasten Seat Belt” sign coming on, turbulence manifests itself in profound ways in science and engineering. A better understanding of turbulent flow could enable radical, more efficient airplane designs and improve prediction in other fields where chaotic flow comes into play, from the human bloodstream to weather forecasting. Researcher Karthik Duraisamy and colleagues at the University of Michigan are using an advanced supercomputer system developed in partnership with IBM to establish a better understanding of a wide range of applications including turbulent flows, advanced materials, climate science and cosmology. The advanced computing system is unique in the sense that it is designed to handle traditional supercomputing with data-intensive operations. One project, conducted in partnership with NASA, combines large amounts of data from wind tunnel experiments with sophisticated simulations to help understand how new wing or engine configurations will perform.

TEEING UP A BETTER GOLF BALL

Working on your golf swing? How about taking a closer look at that ball? Nikolaos Beratlis and Kyle Squires of Arizona State University and Elias Balaras of George Washington University are tapping the power of high performance computation to study how changing the pattern of dimples on a golf ball can change how the air flows around it. Through highly detailed computer simulations using 5 billion points around the surface of a golf ball, the researchers were able to look for insights on how different dimpling changes the air flow pattern and affects the ball’s performance.

Next, the team plans to simulate what happens when the golf ball rotates through the air to better understand how these factors affect a ball’s behavior in real-world conditions.

Dimple technology has non-golf applications as well, from sports equipment to airfoil design and wind turbines.
Energizing Industrial Innovation

Computation is key to investigating intricate chemical, biological and physical processes. Discoveries in these areas translate into new and improved manmade materials and sources of energy.

BIOFUELS YOU CAN FARM

Cellulose—the compound that makes up the fibrous, inedible parts of plants and algae—is the most abundant source of renewable energy on Earth. Although biofuel technologies have improved in recent years, efficiently converting cellulose into useful forms such as sugars and biofuels at industrial scale remains a considerable challenge.

For help, researchers are turning to natural enzymes, such as those found in bacteria and fungi. Finding an enzyme capable of rapidly breaking down cellulose could provide the key to developing inexpensive, efficient methods for large-scale production of cellulose-based fuels.

In a partnership between the Cornell University Center for Advanced Computing and the Texas Advanced Computing Center, Ludmilla Aristilde and her Cornell colleagues have created the first fully computational model that simulates how the chemistry of the solution in which this reaction takes place can interfere with how the enzymes break down cellulose. The simulation (shown at left) helps researchers evaluate candidate enzyme structures that can be designed to optimize the conversion process.

DISCOVERING NEW LEVERS TO CONTROL HEAT AND SOUND

Computer simulations often complement direct experimentation to reveal surprising new discoveries. When Wolfgang Windl, professor at The Ohio State University, ran thousands of simulations of materials in magnetic fields at the Ohio Supercomputing Center, his models suggested that phonons, the atomic vibrations that carry sound and heat, have magnetic properties in all materials. Investigating this phenomenon in the context of a semiconductor material (which is used to build electronic components), a team led by Windl’s colleague Joseph Heremans found that a magnetic field can reduce the amount of heat flowing through the semiconductor by 12 percent.

The history of electronics shows that finding new ways to externally control properties inevitably opens new possibilities for devices. Discovering the pressure sensitivity of electrical current and electrical current created by light, for example, enabled the development of touch screens and solar cells, respectively. Besides being a completely new physical phenomenon, the ability to use magnetic fields to control heat and sound in any material—even non-magnetic ones like wood or plastic—opens intriguing new opportunities for potential applications. This image was created by R. L. Ripley, with contributions from O. Restrepo, N. Antolin and W. Windl.
CRYSTALLIZING UNDERSTANDING OF THE QUASICRYSTAL

Ever since the discovery of quasicrystals (recognized with a Nobel Prize in 2011), researchers around the world have been perplexed by these unique formations of atoms packed in unrepeatable patterns. To study the structure and dynamics of quasicrystals, University of Michigan researchers Michael Engel, Pablo Damasceno and Sharon Glotzer applied high performance computing to model a self-creating quasicrystal with symmetries similar to the protein shells of many viruses. The results revealed a 3-D structure with one of the most complex arrangements of particles ever observed.

Understanding the properties of quasicrystals could help researchers design new types of nanomaterials or “soft matter,” a category of materials that includes liquids, gels and foams. These materials have virtually unlimited applications—such as adhesives, detergents, surgical equipment, paints, and food and fuel additives, among many other uses—and quasicrystals could enhance these materials with useful new properties. A deeper understanding of the behavior of quasicrystals could also lead to new materials capable of turning heat into usable energy.

IN SEARCH OF THE UNBREAKABLE NANOMATERIAL

Nanomaterials offer exciting new possibilities for the future of materials engineering. Created with extremely tiny components, they have unique physical, optical and electrical properties that make them useful for a wide variety of potential applications. One important area of uncertainty, however, is how strong they are.

This image shows an “equilibrium map,” a schematic of how a load-bearing nanoslab of compressed nickel would be expected to behave over time. The perfectly flat structure seen at the bottom gradually develops areas of instability as more weight is applied. By predicting which nanostructures will remain stable under load-bearing conditions, simulations like this can help to inform the design of stronger nanomaterials. The project is a collaboration between Ellad B. Tadmor, Subrahmanyam Pattamatta and Ryan Elliott of the University of Minnesota and Timothy Germann of the U.S. Department of Energy’s Exascale Co-Design Center for Materials in Extreme Environments.

OPTIMIZING COOLANTS FOR A HOT TECHNOLOGY

Helium may be best known as the stuff of party balloons, but it’s playing an important role in one of the world’s hottest technologies: nuclear reactors. Nuclear power today provides about 20 percent of the U.S. power supply, and engineers are constantly tweaking the design of nuclear reactors to optimize safety and efficiency. At the cutting edge of this field is a design concept known as Very High Temperature Reactors (VHTRs), a type of reactor with exit temperatures of up to 1,000 degrees Celsius that is theoretically capable of generating large quantities of energy with essentially zero emissions.

Helium has potential as a coolant for VHTRs because it is an inert gas that does not become radioactive. This simulation, developed by Mark Kimber of Texas A&M University and Anirban Jana of the Pittsburgh Supercomputing Center, shows the changing temperature of helium as it flows through the reactor core. Through a better understanding of how helium will behave in VHTRs, the researchers hope to improve reactor design, creating a new generation of nuclear reactors that is safer, more efficient and easier to maintain.
MAPPING THE BRAIN

Neurological disorders can affect everyone from infants to the elderly, and their impacts can be devastating. On the theory that a better understanding of the brain’s intricate wiring can reveal ways to prevent or correct these problems, researchers are working to map the billions of neural pathways that make up the human brain.

University of Michigan researcher Ivo Dinov is leading an effort to create a 3-D “brain atlas,” visualized at left above, by combining brain images from several clinical, genetic and phenotypic sources. By allowing researchers to virtually navigate multiple sources of information in one cohesive interface, this approach can spark new insights into the anatomy, function and physiology of specific areas of the brain. To help advance general brain research, provide clinical decision support and explore individualized treatments for a wide range of neurological problems, Dinov’s team is constructing individualized and population-based brain atlases using data from patients and healthy volunteers.

Computational neuroscientist Franco Pestilli at Indiana University is developing innovative methods to map brain networks at scale. Pestilli’s laboratory uses multidimensional methods and high-throughput computing to chart millions of brain connections in thousands of living human brains. By charting the macro anatomical properties of the brains of many individuals, the research aims to identify how and why different brains show different properties and inform detection of diseases such as Alzheimer’s or traumatic brain injury. The visualization above right, created by Pestilli in collaboration with Mike Jackson, shows the 3-D structure of a brain network in a living person. Such visualizations can provide researchers and doctors with more precise tools to understand neurological disorders and improve prediction, prevention and treatment—an approach referred to as “personalized neuroscience.”

The Pestilli Lab utilizes Indiana University’s supercomputing facilities in collaboration with Robert Henschel, Arvind Gopu, Sochi Hayashi, Le Mai Liwag Nguyen and Craig Stewart.
THE TECHNOLOGY THAT CHANGED HISTORY

The transition from mobile groups of hunter-gatherers to permanent agricultural settlements was perhaps one of the most influential events in human history, indelibly altering not only how we live but how we influence the world around us. Yet much about this key transition has remained a mystery.

Sean Bergin of Arizona State University uses ASU’s Research Computing resources to simulate how agricultural practices might have spread across the western Mediterranean. Through an approach known as agent-based modeling, the simulation tracks the spread of agricultural villages, incorporating factors such as population growth, group behavior, the spread of ideas, and maritime activity to identify the approximate year, represented with different colors, in which agriculture was likely to have reached a given area.

Using high performance computing to test hypotheses about the lives of early humans could help us piece together our history and gain new insights on human health, culture and socio-ecological change.

VIRTUAL DESIGNS FOR REAL-WORLD CURES

Designing a medical device such as a pacemaker involves juggling numerous complex variables. You not only have to make sure the device will work in different types of bodies and under many circumstances, but that it will be practical to use in a clinical setting and continue to work over a long period of time.

A team led by Arthur Erdman of the University of Minnesota’s Interactive Visualization Laboratory has leveraged the university’s supercomputing resources to create a simulation that allows engineers, designers and medical professionals to collaborate on new medical device designs. Using the simulation, teams can iterate on designs and test new ideas in minutes rather than months, potentially reducing the need for extensive testing in laboratory animals and patients. By streamlining the path from drawing board to operating room, the team hopes their simulation can deliver innovative new devices to patients and save lives in the process. Here, users explore how a cardiac lead for a pacemaker will interact with human anatomy, blood flow and scar tissue formation during a typical lifecycle of the device.

BREATHING NEW LIFE INTO THE STUDY OF ANCIENT ARTIFACTS

The burial rituals of ancient Egypt have been a focus of scientific study for more than a century, yet researchers are still making surprising new discoveries. With help from the Berkeley Research Computing system, Rita Lucarelli of the University of California, Berkeley, is turning photographs of ancient Egyptian coffins, with their heavily detailed markings, into 3-D, fully annotated models. This enables the research team to view the coffins from every possible angle at once, rather than combing through thousands of photographs to find the right image. The project allows researchers around the world to access detailed models of Egyptian artifacts for new insights on burial practices and beliefs about death, magic and the afterlife. Lucarelli’s team also helped uncover and identify previously unidentified coffins kept in the storage rooms of the Hearst Museum of Anthropology at the University of California, Berkeley. They found, for instance, that one of the coffins studied for the 3-D modeling seems to be related to a second, outer coffin belonging to the same mummy.

Here, users explore how a cardiac lead for a pacemaker will interact with human anatomy, blood flow and scar tissue formation during a typical lifecycle of the device.
Waves of Change

From raindrops to oceans, water is at the heart of many climate processes. As our blue planet undergoes large-scale change, researchers are applying high performance computation to understand and adapt to increased flooding, drought and uncertainty.

SAVING THE ‘RAINFORESTS OF THE SEA’

Coral reefs are beautiful as well as functional. Home to an astounding abundance of marine life, they are a key component of the ecosystems that support our fisheries and the marine food web more broadly. They also protect islands and coastlines by absorbing wave energy. Yet these ‘rainforests of the sea’ are increasingly threatened by rising ocean acidity and temperatures, disturbances from fishing and tourism, and the influx of sediments and nutrients from human activities.

The image at top left, an output from a computer-aided visualization developed by Matthew Reidenbach of the University of Virginia, reflects the flow of water through and around a coral reef. By studying how waves, tides and storms affect water flows in coral reefs, researchers are gaining insights on the dispersal of nutrients, sediments and larvae throughout these ecosystems, providing important information to design conservation and reef restoration efforts.

At the National Center for Atmospheric Research, Joan Kleypas and Frederic Castruccio are modeling the complex oceanographic circulation around the Great Barrier Reef and in the Pacific Ocean region known as the Coral Triangle. The Great Barrier Reef has recently experienced the most severe coral bleaching event in recorded history, decimating the reef’s productivity and underscoring the urgency of reef conservation efforts in this region of incredible marine biodiversity. The newly developed high-resolution ocean model is used to understand how larvae from one reef can re-seed reefs in other areas, helping to maintain a healthy reef or replenish one that has become degraded. The image at top right shows the region’s intricate topography and the associated complex turbulent flow patterns that play a critical role in the transport of coral larvae.
PLANNING FOR FLOODS

The basic facts of flooding are simple: too much water, all in one place. But there is still a lot we don’t know about the dynamics at work on and below the surface of the soil that influence where flooding will occur, how long the water will stick around, and how structures such as buildings and levees should be built to best protect human life and property. In the image below, Mississippi State University researcher Bohumir Jelinek develops computational models that track the behavior of large-scale particles to reveal how solids and fluids interact at the nanoscale. Simulating the flow of millions of particles of soil and fluids during a flood, these complex, 3-D models can be used to determine key properties that can help levees and buildings withstand the power and pressure of moving water. The models can also be applied in the context of other situations where fluids meet solids, such as erosion, or industrial processes that involve fluid injection.

UNDERSTANDING OCEAN DYNAMICS—AND OUR FUTURE CLIMATE

The temperature and salinity of the world’s oceans are undergoing dramatic shifts as the planet’s climate changes. These shifts, in turn, cause further changes in weather patterns and global climate, and also influence many aspects of human health, fisheries, and life along the coasts.

These images at right are part of a collaboration between Princeton University and NOAA’s Geophysical Fluid Dynamics Laboratory, led by Princeton researcher Eliot Feibush, to better understand and predict climate changes and impacts. To produce the top image, the team combined bathymetry and sea surface data to model ocean temperature patterns in the winter of a model year. The red streak across the middle of the Pacific Ocean reflects the La Niña weather pattern, which has a strong effect on global climate. The bottom image shows sea surface salinity patterns in the summer of the same model year, revealing flows of low-salinity water (represented in light brown) from melting sea ice in the Arctic and discharge from rivers along the coasts.

PLANNING FOR DROUGHT

Thanks to careful planning and strategic water management, the desert city of Phoenix, Arizona has managed to maintain a reliable water supply despite its famously hot, dry weather. But climate change, increased drought and budget troubles are now challenging the sustainability of the city’s water supply. David Sampson and Ray Quay, researchers at the Decision Center for a Desert City at Arizona State University, have developed a sophisticated computer model for research, teaching and educational outreach around this issue. The model, called WaterSim 5, can be used to examine how various factors interact to influence water supply and water demand. The model takes data from many sources, typically collected separately, and combines them, enabling users to explore different scenarios and see how certain policy decisions or changing environmental conditions would affect water availability. Shown above is the model’s web-based user interface.
Space Science with a Magnetic Appeal

Probing the Invisible Pull of Black Holes
Black holes form when matter is squeezed so densely and gravity pulls so strongly that no particles can escape—not even light. Although they would not be visible on their own, the gas they consume gets extremely hot as it is sucked into the black hole, producing large amounts of radiation. Black holes have attracted considerable attention from researchers hoping for new clues about the cosmos.

This image at top left is from a simulation of the jets that supermassive black holes produce as they accumulate material. Alexander Tchekhovskoy and colleagues at the University of California, Berkeley developed the simulation to investigate what causes the black holes to produce jets (magnetic swirls in a spring-like shape), why they shine, and why they emit bursts of gamma rays.

Scott Noble of the University of Tulsa and Mark Van Moer at of the National Center for Supercomputing Applications at the University of Illinois at Urbana-Champaign created the visualization at top right to study the powerful dynamics at play when two supermassive black holes orbit and merge. This visualization shows the magnitude of the magnetic field (increasing from red to white) in the vertical plane intersecting the orbiting black holes.

A New Appreciation for Earth’s Atmosphere
Without Earth’s atmosphere, we would be bombarded by deadly radioactive particles and ultimately wind up in an unlivable landscape akin to Mars, which has no atmosphere. These images, from a research collaboration between the University of California, San Diego, the University of Leeds and the University of Sheffield, show how the motion of an electrically conductive fluid in a rotating spherical shell generates a self-sustaining magnetic field. The simulation approximates the conditions that are thought to generate the magnetic fields of planets and stars—including the magnetic field that keeps Earth’s atmosphere intact.

Magnetism is a potent force at play in the far reaches of the universe and right here on our home planet. Studying this fundamental force can not only shed light on our natural surroundings but also inform new ways to apply the power of magnetism and gravity for practical applications, from GPS to industrial processes.

Pumping Iron (into the Universe)
Type 1a supernovae are two-part cosmic bodies thought to give the universe most of its iron, including the iron found on Earth and in our own blood. Doron Kushnir of the Institute for Advanced Study in Princeton, New Jersey and David Bock of the University of Illinois, Urbana-Champaign, developed this visualization to address the long-standing question of how 1a supernovae form. Simulating two white dwarf stars directly colliding at thousands of kilometers per second, the model suggests that such an event could cause a thermonuclear explosion and result in a new type 1a supernova.
Arizona State University, ASU
Research Computing
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Providence, Rhode Island

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

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Ithaca, New York

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Berkeley, California

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

Michigan State University, High Performance Computing Center
East Lansing, Michigan

Michigan Technological University
Houghton, Michigan

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

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Bozeman, Montana

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

Oklahoma State University, High Performance Computing Center
Stillwater, Oklahoma

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Piscataway, New Jersey

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Los Angeles, California

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

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University of Miami
Miami, Florida

University of Michigan, Advanced Research Computing (ARC)
Ann Arbor, Michigan

University of Minnesota, Minnesota Supercomputing Institute for Advanced Computational Research
Minneapolis, Minnesota

University of Nebraska, Holland Computing Center
Omaha, Nebraska

University of Nevada, Las Vegas, National Supercomputing Institute (NSI)
Las Vegas, Nevada

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

University of New Hampshire, Research Computing Center
Durham, New Hampshire

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

University of North Carolina at Chapel Hill
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, Advanced Research Computing Services (ARCS)
Charlottesville, Virginia

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

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

Virginia Tech, Advanced Research Computing
Blacksburg, Virginia

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Photo: Sean Cunningham, TACC.