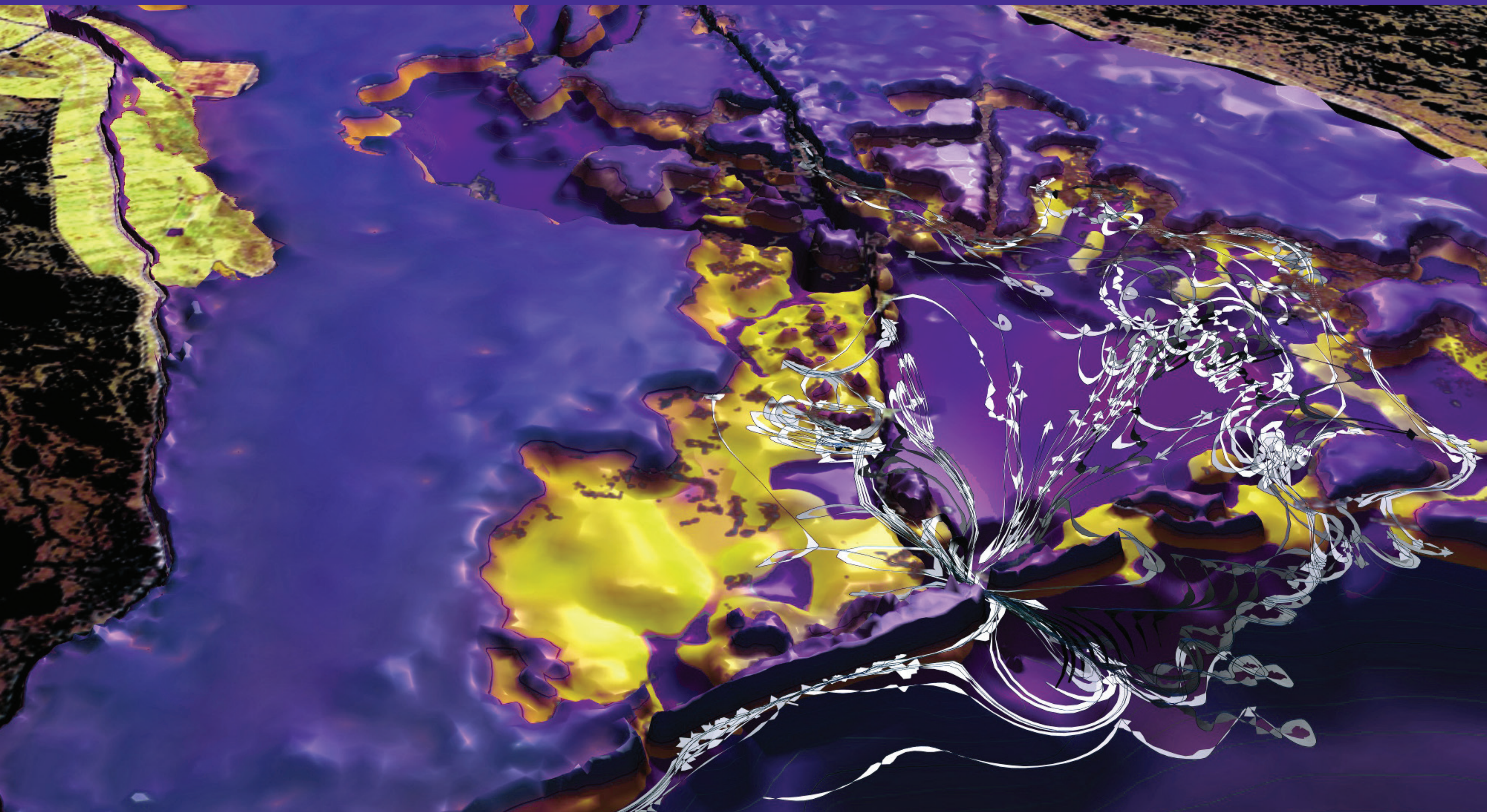
2013

LSU | Center for Computation & Technology

Interdisciplinary I Innovative I Inventive

COMPONENTS

VOLUME 9



Celebrating Another Year Of Success

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Image Credit: LSU University Relations


2013

LSU'S VISION FOR RESEARCH

Kalliat T. Valsaraj
LSU Vice Chancellor of Research & Economic Development

The Office of Research & Economic Development invested significant time and attention to developing a strategic approach to LSU's research, focusing not just on where we are now, but also planning for where we'd like to be. One of our goals is to facilitate more multi-disciplinary, cross-campus research activities. At the same time, we will also work toward increasing LSU's number of international partnerships and further developing existing ones we have in Asia, South America and Europe. These efforts, among other initiatives including increased biomedical and biotechnical research and additional Big Data capabilities, are just a few examples of our vision for LSU's path to success.

LSU's Center for Computation & Technology embodies the spirit behind these efforts, and is certainly helping the University gain more recognition on the state, national and international levels. I'm proud of the accomplishments CCT has gained, and look forward to the new heights this center will most certainly achieve in the near future.

Sincerely,
Kalliat T. Valsaraj

Image Credit: LSU University Relations

Joel Tohline
CCT Director
Alumni Professor, Department of Physics & Astronomy

2013 has been a very successful year at LSU's Center for Computation & Technology.

Through our efforts to attract researchers with an affinity for interdisciplinary collaboration into faculty positions, CCT has established a broad partnership across LSU's academic disciplines. In the summer/fall 2013, 10 new faculty joined LSU in 9 departments because they recognized that the CCT offers a unique environment in which to nurture their research and creative activities.

In August we moved into our new home, the brand-new Digital Media Center, on the campus lake near the corner of South Stadium Drive and E. Parker Blvd. We are glad this moment is finally here. This facility contains advanced classrooms, a recording studio, a theater with a voice lift Constellation system, a machine room housing high-performance computers, technology research labs, and an abundance of research offices interspersed with open and inviting collaborative spaces.

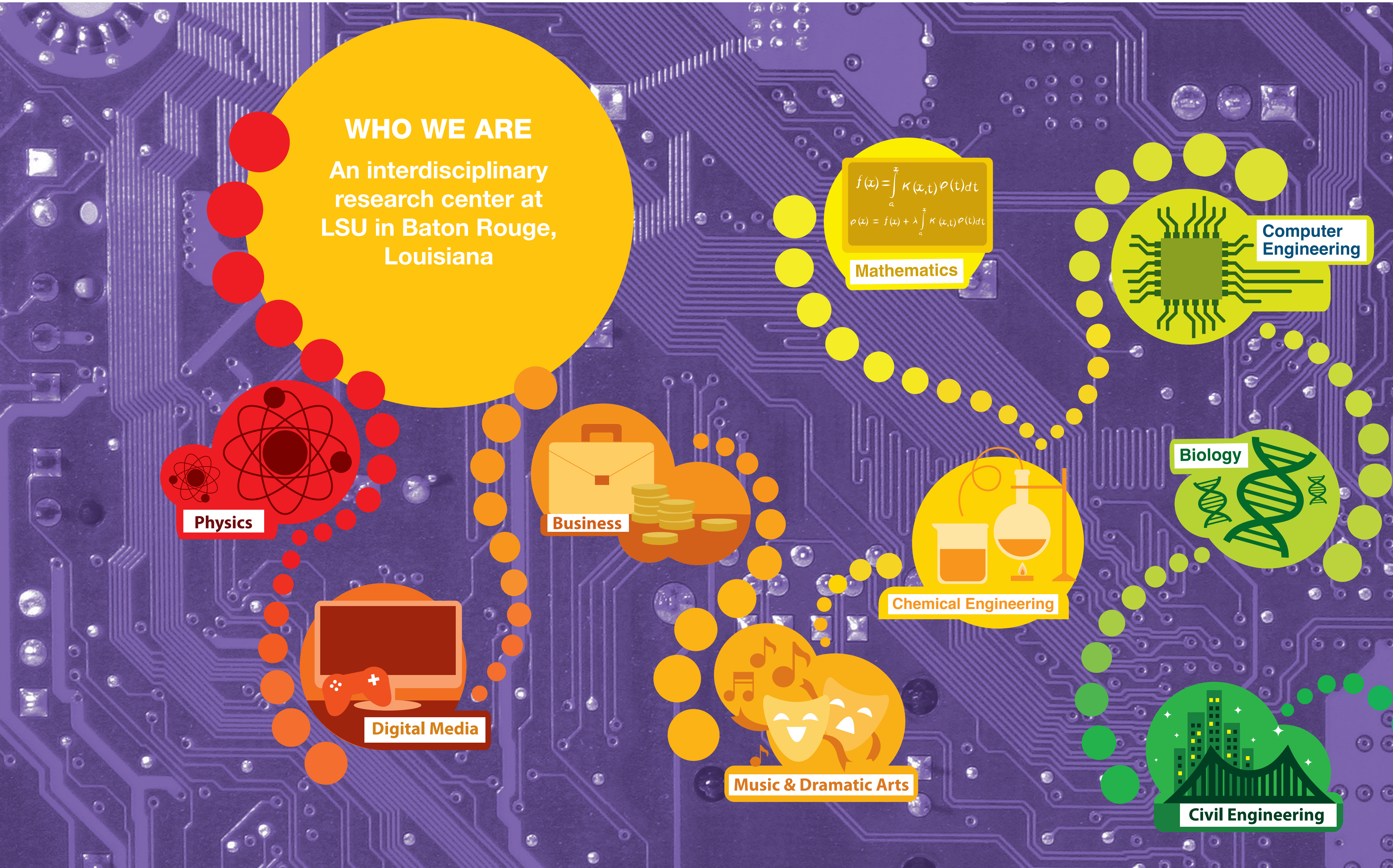
This year has seen significant advancements in research and cyberinfrastructure at CCT. Some recent examples are a $1M NSF grant supporting Big Data Research, and a $4M NSF grant to build the 'SuperMIC' supercomputer.

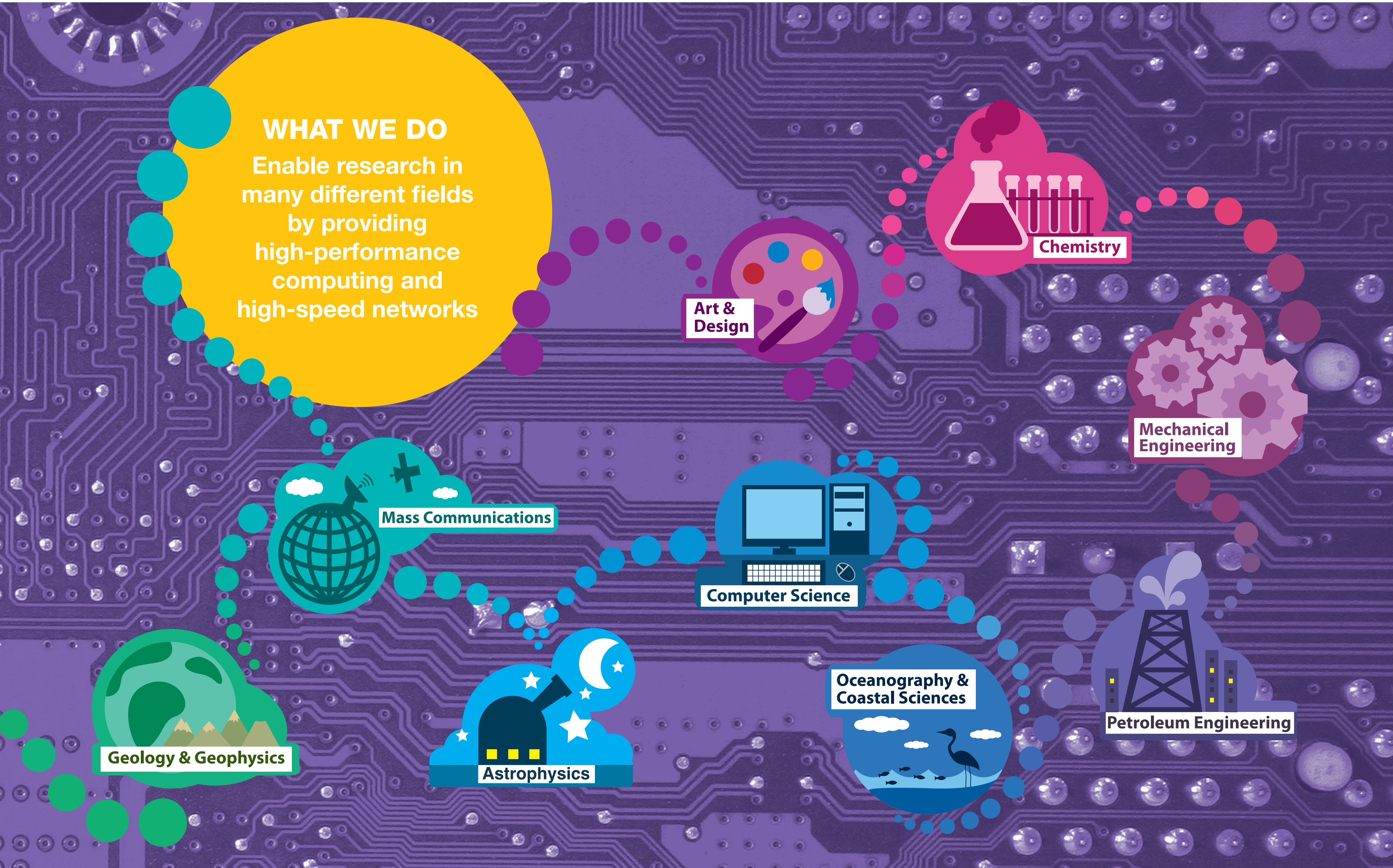
We have had tremendous success initiating a Digital Media Arts & Engineering master's degree program in collaboration with LSU's College of Engineering. This summer we hired Marc Aubanel, a professional with 14 years of executive-level experience with Electronic Arts in Vancouver, B.C., to lead the program that is scheduled to admit its first students in the fall of 2014.

We look into the future with confidence, and we treasure our past. I am pleased to present to you CCT's 2013 annual report. Among other topics, it elaborates on our research and cyberinfrastructure highlights, outlines some of our education and outreach initiatives, and features an industry relations success story.

Sincerely,
Joel Tohline

DISCIPLINES WE TOUCH




WHAT WE DO
Enable research in many different fields by providing high-performance computing and high-speed networks
Art & Design
Chemistry
Mechanical Engineering
Mass Communications
Computer Science
Geology & Geophysics
Astrophysics
Oceanography & Coastal Sciences
Petroleum Engineering

OUR FOCUS AREAS

COAST TO COSMOS

Uses computational fluid dynamics techniques to more accurately anticipate flooding levels associated with hurricanes, to improve coastal ecological forecasting, to simulate extraction of gas and oil from underground reservoirs, and to identify the gravitational-wave signature of merging binary black holes.

CORE COMPUTATIONAL SCIENCE

Research focuses on the development of software algorithms and hardware to enable analysis of a broad array of complex problems on high performance computers and across high performance networks.

CULTURAL COMPUTING

Explores how computational technologies can engage the arts, humanities, and social sciences; and how cultural perspectives impact and transform STEM disciplines. Examples include digital arts and expression, technology adoption,and interactive computational STEAM.

MATERIAL WORLD

Promotes interactions among research groups in the computational fields of materials science, chemistry, and systems biology, all of which rely heavily on molecular dynamics and related numerical techniques.

SYSTEMS SCIENCE AND ENGINEERING

Develops scalable programming models, compilation and runtime techniques, operating systems, and computer architectures in preparation for the new generation of computer systems required for breakthrough applications in science and informatics.

OUR MILESTONES

2001

Gov. Murphy J. “Mike” Foster asks the Louisiana Legislature to appropriate funds as a commitment to the Vision 20/20 plan specifically for Information Technology development. The Legislature authorizes $25 million, with $9 million going to LSU. The University creates the Center for Applied Information Technology and Learning (LSU CAPITAL) to improve information technology on campus. LSU Department of Physics & Astronomy Professor Joel Tohline serves as interim director.

2002

LSU, through LSU CAPITAL, acquires its first supercomputer, named SuperMike. At the time, SuperMike is the second-fastest computer among academic institutions worldwide.

2003

LSU hires world-renowned astrophysicist Ed Seidel to implement his vision for a fully interdisciplinary research center as LSU CAPITAL’s director. The center is renamed the LSU Center for Computation & Technology, or CCT.

2004

Gov. Kathleen Babineaux Blanco commits $40 million throughout a 10-year period to fund the Louisiana Optical Network Initiative, a high-speed, fiber optic network that connects supercomputers around the state for increased research collaboration and economic development potential. CCT Director Ed Seidel co-authored the white paper that envisioned LONI and how it would benefit Louisiana.

2007

CCT and LSU Department of Computer Science Professor Thomas Sterling premiers his High-Performance Computing: Models, Methods, and Means course. This course is the first of its kind in the United States, broadcasting the lessons in high-definition video across high-speed networks to four other universities in Louisiana, around the country, and internationally.

2008

Stephen Beck and Jorge Pullin appointed as interim co-directors of the CCT while the University undertakes an international search to find a permanent CCT director.

2010

November:
Researchers at CCT, together with several other universities across Louisiana, received $20 million from the National Science Foundation to create Louisiana Alliance for Simulation-Guided Materials Applications, or LA-SiGMA. This is one of the state's largest grants ever from NSF.

December:
LSU announced that Alumni Professor Joel Tohline was named the new director of CCT. Tohline is an internationally recognized scholar in the fields of astrophysics, computational fluid dynamics, and scientific visualization and in all respects is a computational scientist and user of high performance computing.

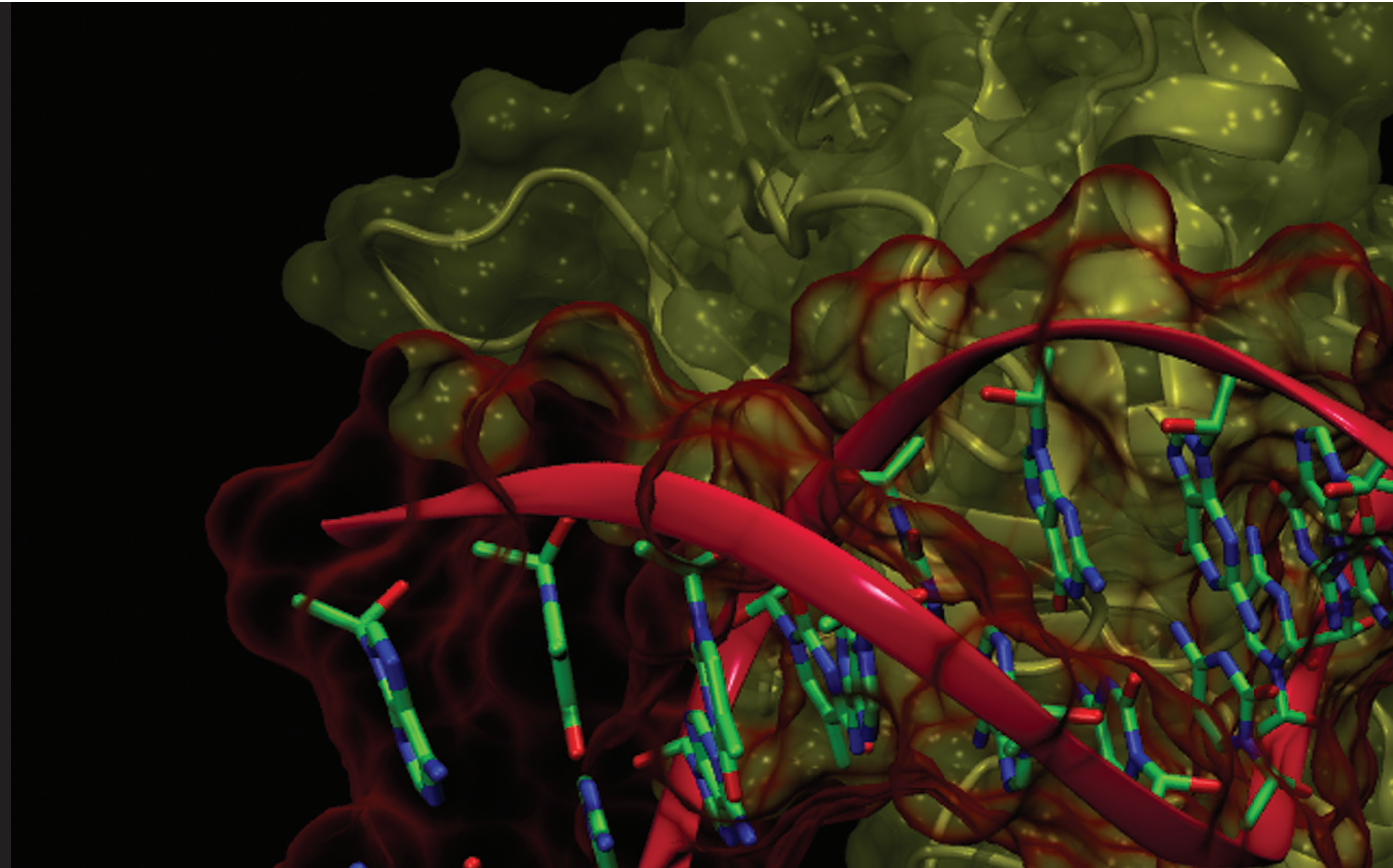
2012

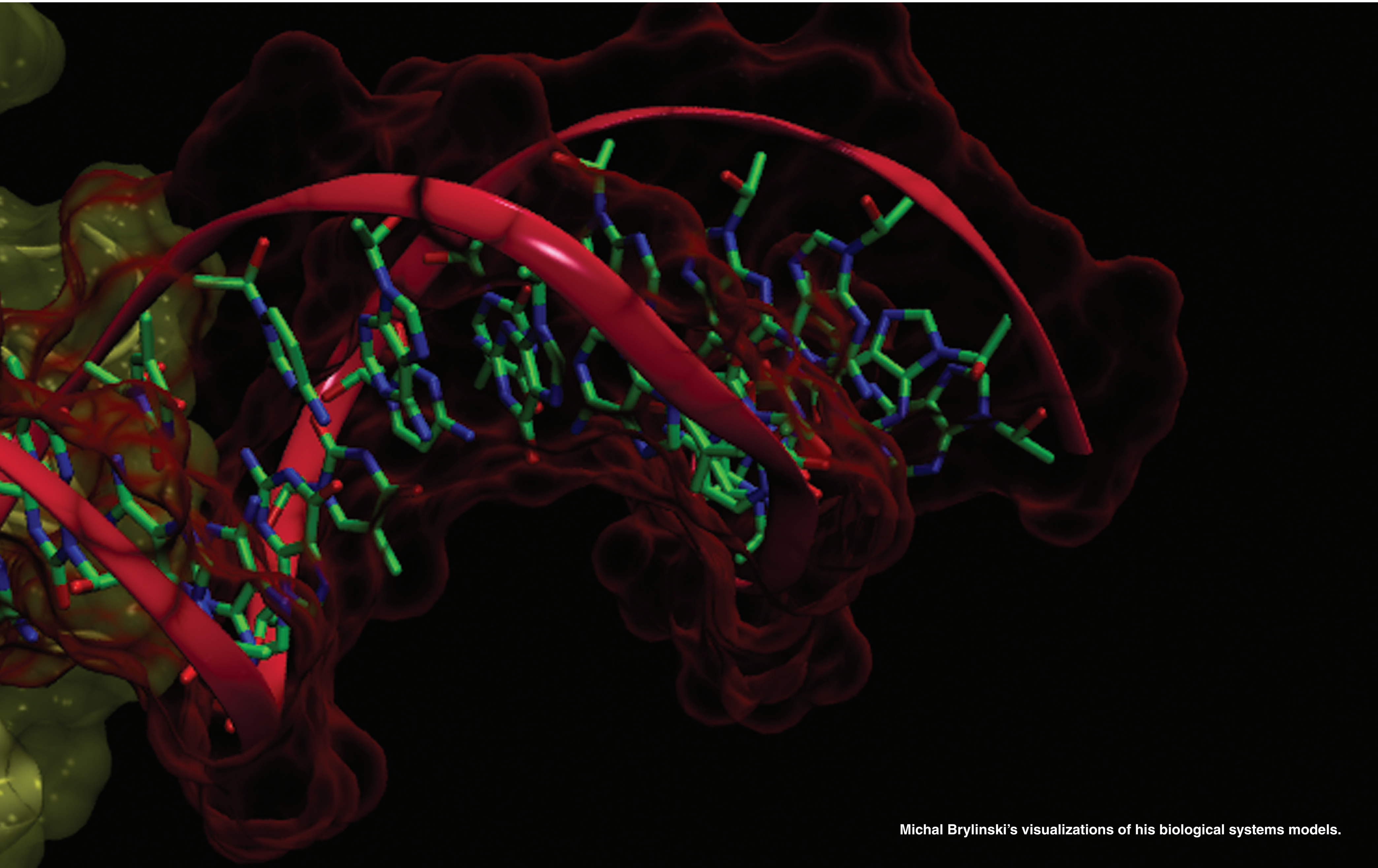
CCT was named a 2012 CUDA Research Center by NVIDIA.

2013

CCT moves to the brand-new Digital Media Center.

RESEARCH FACULTY





Michal Brylinski's visualizations of his biological systems models.

WE CONDUCT RESEARCH TO DESIGN BETTER MATERIALS WITH GREATER FUNCTIONALITY

By Tatiana Johnson

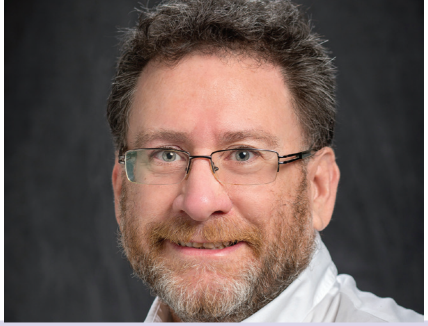
New-generation batteries, synthetic fibers in bullet-proof clothing, substitutes for critical minerals, more effective medication, packaging that would keep food fresh longer—advanced materials are a part of our everyday lives. The field of materials by design uses high-performance computing to model, create, and develop such advanced materials.

LSU CCT is an ideal environment for scientists to conduct advanced materials research.

CCT's Material World focus area unites faculty from departments such as physics & astronomy, math, biological sciences, chemistry, chemical engineering, computer science, and geology & geophysics, who explore novel approaches in materials science. Unlike the traditional model, "given the material, find the property," the new approach follows the model "given the property, find the material."

"We are working towards developing better materials with greater functionality," said Mark Jarrell, Material World focus area lead and a professor in

Superconductivity is of special interest to CCT's Material World Focus Area. The image depicts a magnet levitating above a high-temperature superconductor, cooled with liquid nitrogen.



Mark Jarrell
Department of Physics & Astronomy
CCT Material World Focus Area Lead

Juana Moreno
Department of Physics & Astronomy
CCT Material World Focus Area

LSU's Department of Physics & Astronomy.

"Whether it's for power transmission through superconductors or faster computer chips, we want this work to lead to materials that the industry can use to develop better technology for areas such as electronic devices, medical science—even magnetic levitation trains," Jarrell said.

"To design materials with specific behaviors and functions, we need to accurately describe the physics and chemistry that's at work," he said. "High-speed computing and high-speed networks that help understand the physics behind a material are becoming more robust, which is helping narrow the design space," Jarrell said.

Knowing what makes one material perform in a particular way might simplify creating a new material with similar properties. And using that knowledge to shorten the path to discovery is an important step on the road to materials by design.

One example of the phenomena the Material World focus area explores is superconductivity. It happens when a substance (typically metallic or ceramic) reaches its critical temperature and loses all electrical resistance. This occurs at extremely low temperatures, which makes it difficult to apply to real-life situations.

Collaborating with Mark Jarrell, Juana Moreno, faculty member in CCT's Material World focus area and an associate professor in LSU's Department of Physics & Astronomy, is trying to better understand the structural changes that create this rare phenomenon. Both of them are exploring how to develop superconductive materials that would work at room temperature. By transporting energy very efficiently, superconductors hold great potential for emerging applications in electronic devices, transportation, and also power transmission, generation, and storage.

"Computational materials is a very coordinated effort in Louisiana," Moreno said. "We are part of the Louisiana Alliance for Simulation-Guided Materials Applications, or LA-SiGMA, that creates a statewide research and education program focusing on three science drivers: electronic, energy, and biomolecular materials."

continued on p.16

Bill Shelton
Department of Chemical Engineering
CCT Material World Focus Area

continued from p.15

Created in 2010, the LA-SiGMA initiative is one of the largest National Science Foundation grants that Louisiana has ever received—$20 million. LA-SiGMA shares the vision of the Materials Genome Initiative for Global Competitiveness, announced by President Obama in June 2011, of developing an infrastructure to accelerate advanced materials discovery and deployment in the Unied States.

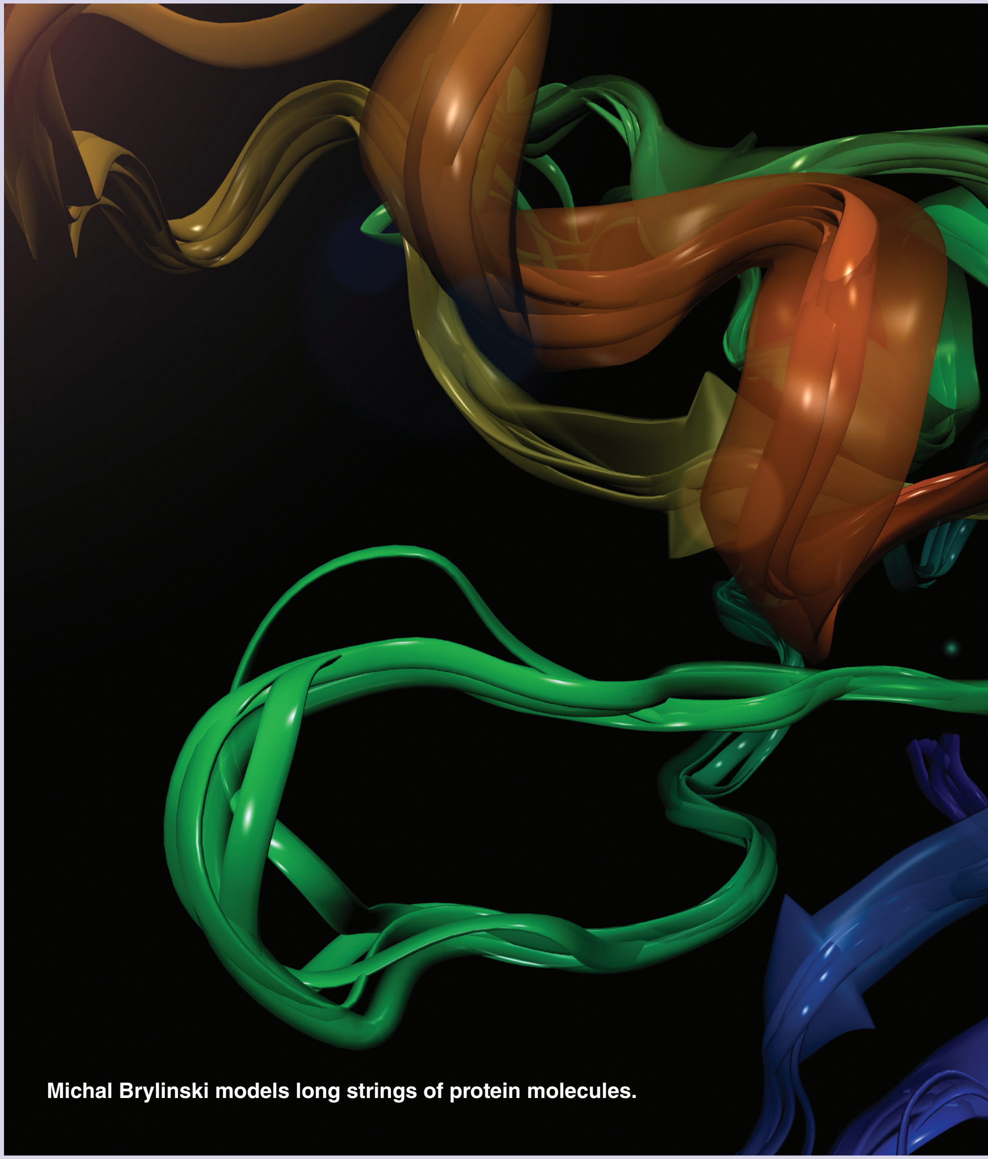
In the fall 2013, four newly hired LSU faculty joined CCT's Material World focus area, because they recognized that CCT offers a unique collaboration.

Among them is Bill Shelton, a nationally prominent materials scientist who was hired jointly by CCT and the Department of Chemical Engineering. Shelton has known Mark Jarrell for a long time and has collaborated with him and Juana Moreno in the past several years while working at Pacific Northwest National Laboratory, a U.S. Department of Energy government research laboratory in Richland, WA. His research area involves advanced materials used in the auto, aerospace, military, and electronics industries.

"Light-weight and high-strength alloy systems are important for applications in the auto industry to lighten the vehicle for better fuel efficiency while maintaining safety," Shelton said. "Another type of materials—light-weight, high-strength, and high-temperature materials—is used in turbine blades for improved fuel efficiency of an airplane as they allow for running the turbine engines at higher temperatures. What's more, these high-strength materials are used for military applications to withstand armaments," he said.

Another CCT new hire, Revati Kumar, who also joined LSU's Department of Chemistry this fall, explores molecular level understanding of electrolyte behavior in rechargeable batteries. Electrolyte is the material that separates anode and cathode, and through which ions are transported. Its degradation can significantly reduce the battery's life.

"To design the next generation of batteries, it is imperative that we understand the factors that reduce their life cycle. My research focuses on electrolyte optimization—an important component of battery systems," Kumar said.



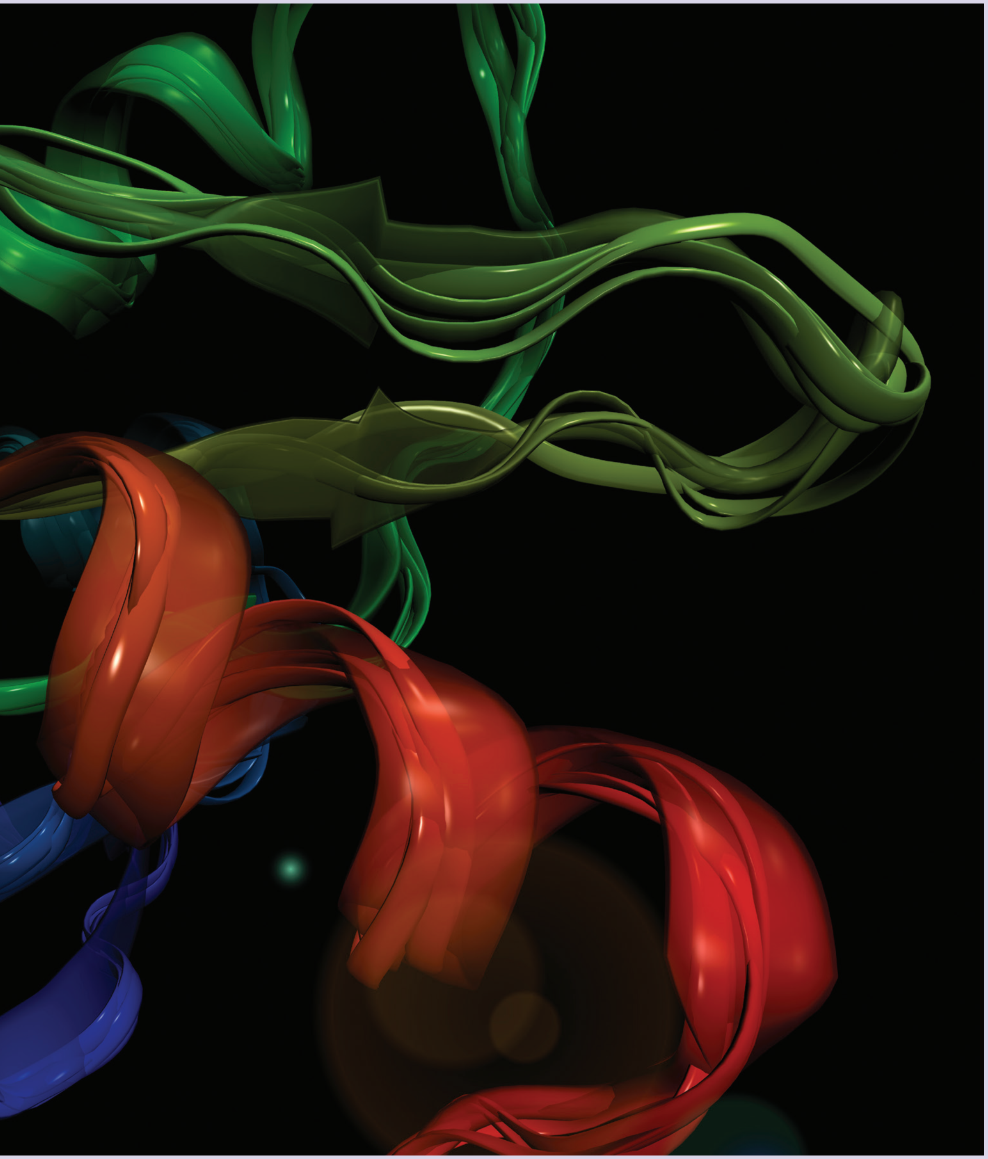
Michal Brylinski models long strings of protein molecules.

Revati Kumar
Department of Chemistry
CCT Material World Focus Area

Kenneth Lopata
Department of Chemistry
CCT Material World Focus Area

Michal Brylinski
Department of Biological Sciences
CCT Material World Focus Area

Jianwei Wang
Department of Geology & Geophysics
CCT Material World Focus Area



Kenneth Lopata joined LSU's Department of Chemistry and CCT this fall, too. He studies electrons and nuclei in motion.

"When light hits matter, it causes electrons, and in turn nuclei, to move, resulting in millionth of a billionth of a second changes in the material," Lopata said. "This extremely fast motion is crucial in materials such as photovoltaics, for example, where light is absorbed by a material and converted to electrical energy," he said.

Advanced materials research not only deals with metals, crystals, and liquids, but can also involve biological systems. CCT's Michal Brylinski, who has a joint appointment with LSU's Department of Biological Sciences, models strings of protein molecules, putting them together in different configurations. This helps him understand how a certain bacteria or a drug connects to the surface of a cell and interacts with it at the atomic level.

"Studying a protein in isolation is not enough, because it interacts with other proteins that could modify its function, so I have to put each protein in a context of a living cell," Brylinski said.

Yet another area where advanced materials research can be applied is Earth science. Jianwei Wang, who joined LSU's Department of Geology & Geophysics and CCT's Material World group this fall, does just that.

"I do molecular modeling to understand properties of geomaterials," Wang said. "The results are used to predict material properties in geological processes. For example, by linking interactions of contaminants (natural or man-made) with rocks in underground water systems to their molecular scale controls at mineral-water interfaces, the transport of the contaminants can be better predicted and the environmental impact can be addressed *a priori*," Wang said.

"All CCT's materials scientists share the need for taking a certain set of mathematical equations and teaching the supercomputer to solve them effectively. The techniques that they use overlap, and this is why the researchers benefit so much from interacting with one another," said CCT Director Joel Tohline. ◆

WE BRING BIG DATA COMPUTATIONAL CAPABILITIES TO VARIOUS RESEARCH GROUPS AT LSU

By Paige Brown

LSU's Seung-Jong Park, associate professor in the Department of Computer Science & Engineering with a joint appointment at CCT, along with co-investigators Joel Tohline, Sean Robbins, Lonnie Leger, K. Gus Kousoulas, and other senior LSU faculty, received a $947,860 National Science Foundation grant for a campus-wide Big Data project. Samsung Electronics is also participating in the project as an industrial collaborator.

The project, titled "CC-NIE Integration: Bridging, Transferring, and Analyzing Big Data over 10Gbps Campus-Wide Software Defined Networks," will empower scientific breakthroughs at LSU by providing researchers with advanced information technologies and cyberinfrastructure.

"Big Data is a very hot term now," Park said. "Genome sequencing is one of the major drivers for Big Data research. It is not unusual to produce many terabytes of data in sequencing the human genome, or trillions of digital information bytes. But processing terabytes of data has been a headache for research-

Seung-Jong Park
Project Pricipal Investigator
Department of Computer Science & Engineering
CCT System Science & Engineering Focus Area

K. Gus Kousoulas
Co-Principal Investigator
ORED Associate Vice Chancellor
Director, Division of Biotechnology & Molecular Medicine

ers using their own equipment." Genome sequencing, which involves determining the exact sequence of an organism's hereditary molecule known as DNA, has many applications in biological and medical research, including personalized medicine.

However, genome sequencing require large amounts of data processing. The human genome, for example, contains three billion molecular units, like three billion beads on a string arranged in a specific order. Assembling this amount of data, or even assembling shorter genome sequences like those of the West Nile and HIV viruses, for example, will require massive computational power and data storage capabilities.

"Right now, with current technology, LSU's supercomputers are not adapted for Big Data," Park said.

But that is set to change. Park and colleagues are building a high-speed intra-campus network that will connect separate lab groups on campus to LSU's primary supercomputer facility.

Samsung is collaborating with LSU on the high-speed network-building phase of the project, helping to establish high-speed networks and large memory storage units on campus in order to handle the massive amounts of data generated by Big Data applications. Samsung has donated 70 terabytes of solid state disk storage to LSU for this project.

"With this network, after researchers produce their data, they could send it over our 10 gigabyte-per-second network to LSU supercomputing clusters," Park said.
The concept is similar to that of cloud computing, where instead of needing their own high-performance computers in the future, LSU researchers will be able to send all of their scientific data over a network to be processed and analyzed automatically by a large number of connected computers across campus.

"The reviewers of this proposal at the national level understand that LSU houses the unusual combination of talents that is required to make complex and innovative projects of this type successful," said Joel Tohline, CCT director. "LSU not only has a diverse group of scientists and engineers that can take advantage of this new capability, but also highly skilled technical staff who can implement the new cyperinfrastructure."

And this is just the beginning. Park sees the potential for extending this Big Data network to Louisiana as a whole, bringing LSU's supercomputing cluster capabilities to research projects at Pennington Biomedical Research Center, Tulane University, and other institutions interested in Big Data.

"The cyberinfrastructure developed at LSU with this NSF funding can serve as a model for facilitating and promoting biomedical and other research collaborations among all LSU campuses and other institutions in Louisiana in the future," said K. Gus Kousoulas, Co-Principal Investigator of the project. ◆

WE EXPLORE QUANTUM GRAVITY THAT TAKES SINGULARITY OUT OF BLACK HOLES

LSU CCT's Jorge Pullin and Rodolfo Gambini at the University of the Republic in Montevideo, Uruguay, showed in their May 2013 article in *Physics Review Letters* that loop quantum gravity eliminates the singularity inside a black hole. The work has been highlighted in a number of international media, including a London-based science and technology magazine, *New Scientist*, as well as in *Indian Express, International Business Times Italia, The Asian Age, TopNews New Zealand, Live Science, Physics Central, Inside Science*, phys.org, and more.

Reprinted from *New Scientist*
May 29, 2013

By Katia Moskvitch

Falling into a black hole may not be as final as it seems. Apply a quantum theory of gravity to these bizarre objects and the all-crushing singularities at their cores disappear.

In its place is something that looks a lot like an entry point to another universe. Most immediately, that could help resolve the nagging information loss paradox that dogs black holes.

"Information doesn't disappear, it leaks out," said Pullin.

Jorge Pullin
Professor and Horace Hearne Chair in Theoretical Physics
Department of Physics & Astronomy
CCT Coast to Cosmos Focus Area

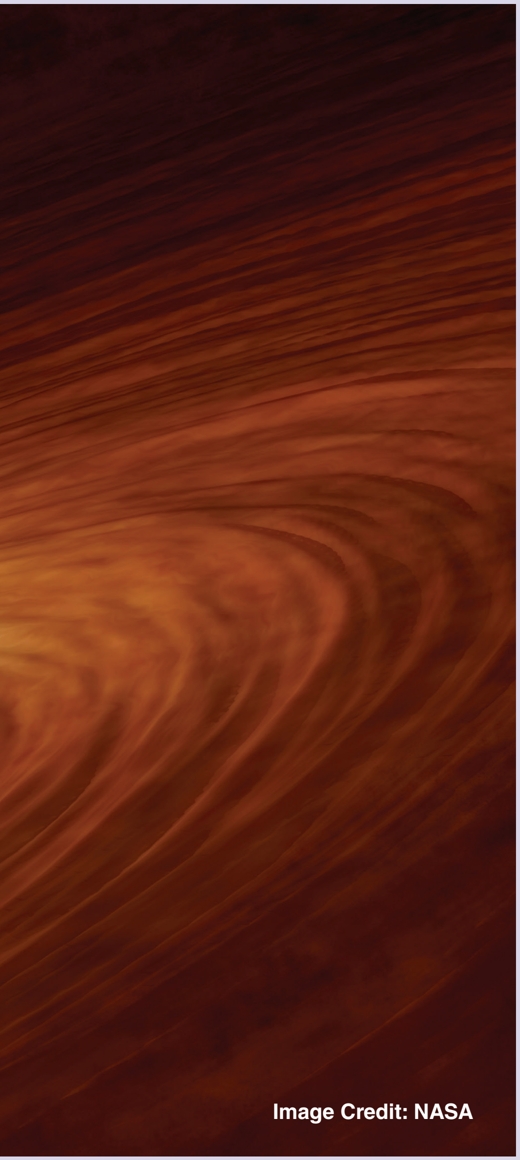


Image Credit: NASA

Though no human is likely to fall into a black hole anytime soon, imagining what would happen if they did is a great way to probe some of the biggest mysteries in the universe. Most recently this has led to something known as the black hole firewall paradox—but black holes have long been a source of cosmic puzzles.

According to Albert Einstein's theory of general relativity, if a black hole swallows you, your chance of survival is nil. You'll first be torn apart by the black hole's tidal forces, a process whimsically named spaghettification.

Eventually, you'll reach the singularity, where the gravitational field is infinitely strong. At that point, you'll be crushed to an infinite density. Unfortunately, general relativity provides no basis for working out what happens next.

"When you reach the singularity in general relativity, physics just stops, the equations break down," said Abhay Ashtekar of Pennsylvania State University.

The same problem crops up when trying to explain the big bang, which is thought to have started with a singularity. So in 2006, Ashtekar and colleagues applied loop quantum gravity to the birth of the universe. LQG combines general relativity with quantum mechanics and defines space-time as a web of indivisible chunks of about 10-35 metres in size. The team found that as they rewound time in an LQG universe, they reached the big bang, but no singularity—instead they crossed a quantum bridge into another older universe. This discovery is the basis for the big bounce theory of our universe's origins.

Now Jorge Pullin at Louisiana State University and Rodolfo Gambini at the University of the Republic in Montevideo, Uruguay, have applied LQG on a much smaller scale—to an individual black hole—in the hope of removing that singularity, too. To simplify things, the pair applied the equations of LQG to a model of a spherically symmetrical, non-rotating "Schwarzschild" black hole.

In this new model, the gravitational field still increases as you near the black hole's core. But unlike previous models, this one doesn't end in a singularity. Instead gravity eventually reduces, as if you've come out the other end of the black hole and landed either in another region of our universe, or another universe altogether. Despite only holding for a simple model of a black hole, the researchers—and Ashtekar—believe the theory may banish singularities from real black holes, too.

That would mean that black holes can serve as portals to other universes. While other theories, not to mention some works of science fiction, have suggested this, the trouble was that nothing could pass through the portal because of the singularity. The removal of the singularity is unlikely to be of immediate practical use, but it could help with at least one of the paradoxes surrounding black holes, the information loss problem.

A black hole soaks up information along with the matter it swallows, but black holes are also supposed to evaporate over time. That would cause the information to disappear forever, defying quantum theory. But if a black hole has no singularity, then the information needn't be lost—it may just tunnel its way through to another universe.

"Information doesn't disappear, it leaks out," said Pullin. ◆

WE OBSERVE THE FOOTPRINTS OF ASTRONAUTS ON THE MOON

By Cassie Thibeaux

It's not everyday that someone other than an astronaut or planetary scientist can observe the footprints of astronauts on the moon.

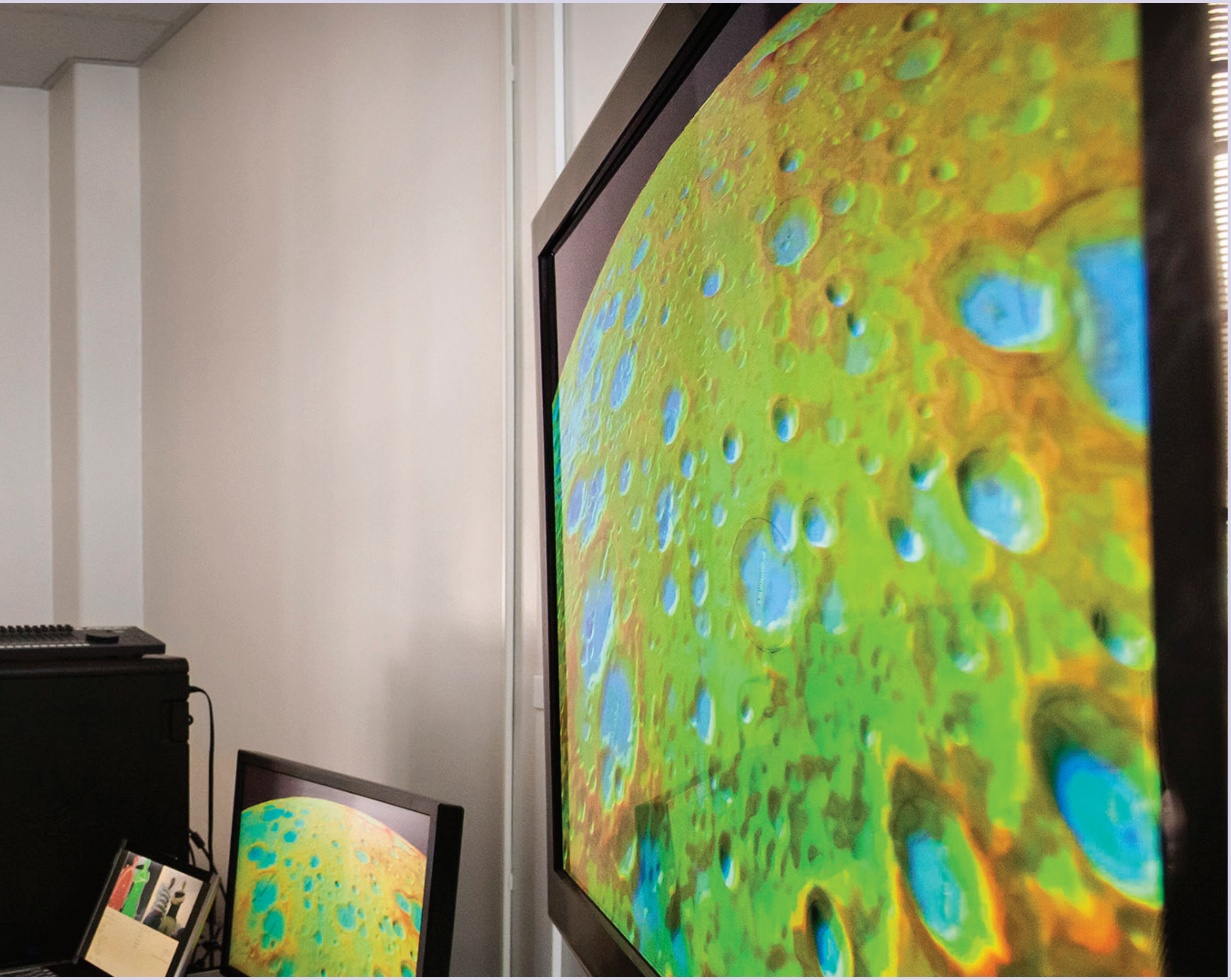
Robert Kooima, assistant professor of computer science in the LSU School of Electrical Engineering & Computer Science and a faculty member at CCT can do just that.

Kooima collaborated on the Lunar Reconnaissance Orbiter Camera, a project funded by NASA to send a new probe to the moon to collect hundreds of terabytes of data.

The scientists were then charged with taking the raw data collected from the probe and distilling, reorganizing, and restructuring it into an interactive format that displayed a believable image of the moon for both children and adults.

Image Credit: LSU University Relations

Robert Kooima
Department of Computer Science & Engineering
CCT Cultural Computing Focus Area



Located at the Adler Planetarium in Chicago, the Moonwall exhibit provides a high-resolution interactive fly-over of the moon and allows visitors to maneuver the moon with a joystick. Kooima hopes to bring a similar exhibit to the Louisiana Art and Science Museum with additional interactive tools, such as a QR code that connects people to the exhibit via a cellphone.

Museum exhibits like the Moonwall aren't always associated with computer scientists, and the field of computer science isn't always easily understandable.

Kooima's research interests—computer graphics and interaction—bridge the disconnect between the academic and practical sides of computer science and help to illustrate the growing importance and relevance of digital media. ◆

WE CONDUCT STE||AR SYSTEMS TECHNOLOGY, EMERGENT PARALLELISM, AND ALGORITHM RESEARCH

By Adrian Serio

STE||AR (pronounced stellar) is a group of CCT faculty, researchers, and students whose work is centered around the new ParalleX execution model and its implementation in HPX (High Performance ParalleX), a modern runtime system. HPX is used for a broad range of system software solutions and scientific applications for hybrid and many-core hardware architectures, helping scientists and developers write code that scales and performs better compared to more conventional programming models such as MPI or OpenMP.

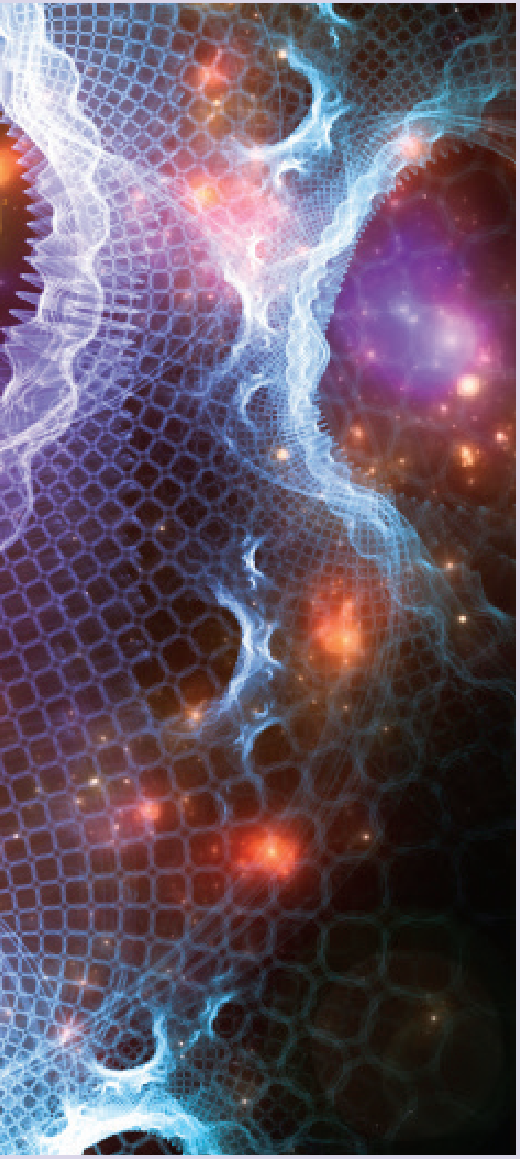
HPX – A Parallel Runtime System for Applications of any Scale

As systems grow to Exa-scale, greater shared resources and the widespread adoption of specialized heterogeneous systems lead to greater hardware complexity. Applications are also becoming more complicated as increasingly dynamic and adaptive methods are required to make use of untapped computing resources.

To keep up with the fast growth of hardware capabilities, new execution models must be developed.

Hartmut Kaiser
CCT IT Consultant
Adjunct Associate Research Professor
Department of Computer Science &
Engineering

Adrian Serio
CCT STELLAR Group Scientific
Program Coordinator



HPX is designed by the CCT STE||AR Group to enable developers to exploit the full processing power of many-core systems with an unprecedented degree of parallelism. It is based on a novel combination of well-known ideas with new and unique overarching concepts.

HPX aims at resolving the problems related to application scalability, resiliency, power efficiency, and runtime adaptive resource management that are of growing importance for the whole scientific computing community. It departs from today's prevalent programming models with the goal to mitigate their respective limitations, such as implicit and explicit global barriers, coarse grain parallelism, and lack of overlap between computation and communication.

Static scheduling and data partitioning solutions—as preferred today—cannot provide the best performance throughout execution. Problems change during execution, as do systems and their bottlenecks. HPX provides tools to enable control and introspection during execution, allowing for the system and the application to flexibly adjust to improve performance.

HPX represents a portable and innovative mixture of a global system-wide address space, fine grain parallelism, lightweight synchronization, and work-queue based implicit message-driven computation. It provides the full semantic equivalence of local and remote execution along with explicit support for hardware accelerators.

Using HPX for Future-Oriented Collaborations

As HPX development continues, the Stellar group has begun to collaborate on transformative projects with many different institutions across the world.

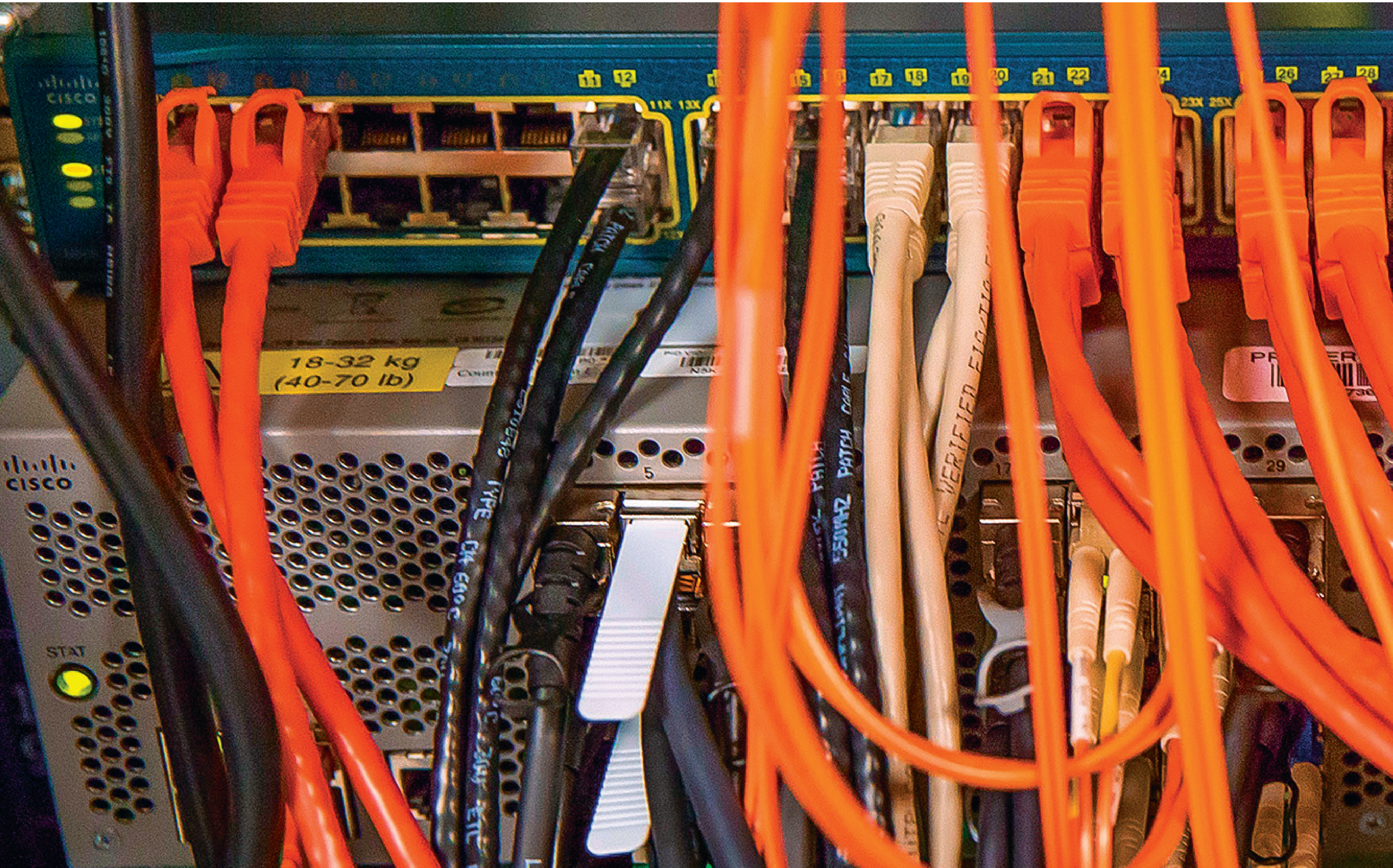
Examples of these partnerships include our international collaborations with colleagues from the Friedrich-Alexander-University in Erlangen (Germany, FAU) and the NSF-funded STAR project, tying together researchers from LSU's Department of Physics & Astronomy and the STE||AR group.

In both cases, HPX is used for developing higher-level application frameworks that help domain scientists leverage the advantages of a new straightforward way of computing in their applications.

In this context, HPX has been successfully integrated with both the LibGeoDecomp (a Library for Geometric Decomposition codes) developed at FAU and the Octopus framework for fluid dynamics simulations developed by STE||AR. The first results gathered from these projects solidly confirm the expectations that the new technology developed by STE||AR will have a high impact on the domain sciences. This research will enable scientists to run their applications with high parallel efficiency at an unprecedented scale.

HPX development has been sponsored, in part, by the NSF (National Science Foundation), DOE (Department of Energy), DARPA, and Microsoft as well as by the CCT. It is central to the DOE funded X-STACK project led by Sandia National Laboratories. More information and means for accessing the HPX libraries may be found at stellar.cct.lsu.edu. ◆

CYBERINFRASTRUCTURE



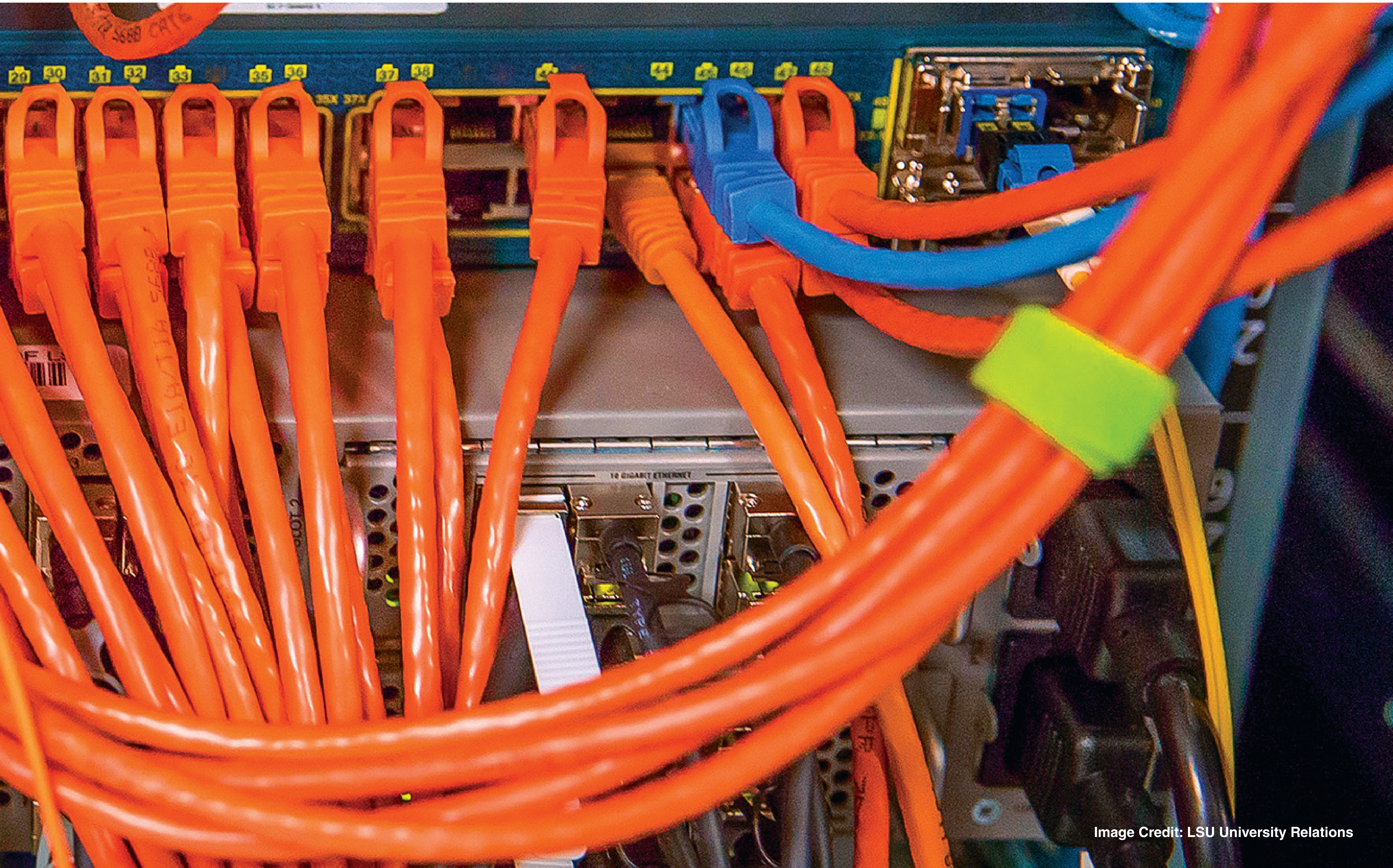


Image Credit: LSU University Relations

WE DEVELOP MELETE, AMONG FIRST INTERACTIVE SUPERCOMPUTERS

By Tatiana Johnson

In today's society, interactivity is a constant buzzword—it is hard to imagine a person who has not seen a smart phone or a tablet. But how about an interactive supercomputer? Not so common.

Since 2011, researchers at CCT have been working to envision what interactivity with these big machines could mean. CCT's Brygg Ullmer, who is also an associate professor of computer science at LSU, is leading a team of some 40 co-investigators across 11 departments in 5 colleges on a ca. $1 million grant from the National Science Foundation to develop Melete.

Melete, named after the muse of practice in Greek mythology, is a system that integrates an interaction-oriented compute cluster with tangible interfaces.

"In the classroom, laboratories, and meeting rooms, faculty today choose between real-time interaction with the limited capability of a laptop or podium PC or no interaction at all," said Melete's principal investigator Ullmer.

"Through Hollywood, everyone is aware of the simulation potentials of large-scale computation. We aspire to bring some of these powers of interactive hurricane simulations, of flowing hair, and animation work to what students and faculty are controlling and experiencing live in the classroom as well as at a research meeting."

CCT's IT consultant and adjunct faculty of computer science Chris Branton has been leading the development of software infrastructure for the project.

"Typically, a high-performance computer would feature one head node coupled with several slave nodes," Branton said. "In contrast, Melete features several interactive face nodes in addition to the head node. These are a combination of dynamic screens, passive printed visuals, addressable LEDs, and other interactive elements. They are planned to be placed in labs, meeting spaces, and classrooms both at CCT and elsewhere at LSU to give interactive control of the machine to authorized users," he said.

Five research domains are expected to benefit from Melete—computational biology, materials, mathematics, engineering, and arts. LSU professor of chemistry Les Butler, who co-leads the project, explained how the new system has helped his research on flame-retardants and X-ray interferometry for materials science.

"This area of research is just a few years old, so our software is under rapid development, and it is a tremendous advantage to use Melete with our new Mathematica codes," Butler said. "The data rate of X-ray imaging is huge—a couple of days yields roughly one terabyte of data. How can we present these results to our collaborators? Melete helps us extract the good stuff," he said.

"As our interface for this project, we are using four iPad minis (one image type per iPad)," Butler said. "It's strange, but it seems to work. We can discover features in the data sets walking to and from the coffee shop that would otherwise tether us to the workstation."

"By the way, X-ray interferometry may soon appear in clinical applications as low-radiation dose imaging. Researchers at the National Institutes of Health are exploring this new X-ray method for applications such as mammography."

Brygg Ullmer
Project Principal Investigator
Department of Computer Science & Engineering
CCT Cultural Computing Focus Area Lead

Chris Branton
CCT IT Consultant
Adjunct Professor
Department of Computer Science & Engineering

Jinghua Ge
CCT Visualization Consultant

Jinghua Ge, a visualization consultant at CCT who is collaborating with Butler on the flame-retardant research, explained how Melete is enhancing her work. "The old-fashioned visualization software is not keeping up with the data growth, and personal computers are just not powerful enough to provide large-scale interactive data exploration. We use the VisIt parallel software to visualize large-scale scientific data on Melete," Ge said.

Landon Rogge, a senior in computer science at LSU, has played an active part of the Melete team as well, facilitating simpler access to the Melete system for scientists who are unfamiliar with command-line interfaces.

"After graduation in May 2014, I plan to apply to the FBI to pursue a career in fighting cyber-crime, which frequently involves the use of HPC systems and other tools I learned on the Melete project," he said.

Who knows, maybe over the next decade, a smart phone will function as a multi-hundred core personal device. Ullmer and the Melete team are certainly moving in that direction. ◆

WE RECEIVE $4M NSF GRANT FUNDING FOR SUPERMIC SUPERCOMPUTER

By Paige Brown

Imagine a giant supercomputer cluster that could do the work of nearly 500 versions of your fastest laptop or desktop computer at home. Now imagine that this supercomputer could take all that computing power and throw it at a single problem—finding a new drug target, for example, or solving equations to find out exactly where Hurricane Katrina's storm surge flooding would fall.

This seemingly far-fetched dream is becoming reality at LSU. Researchers at the CCT have received a Major Research Instrumentation award from the National Science Foundation, or NSF, of nearly $4 million for the acquisition of SuperMIC, a new supercomputer cluster. The machine, which will be harnessed for a variety of research projects involving discovery of new drugs, modeling coastal processes, and forecasting hurricane-generated waves and storm surges, will allow Louisiana to take the next step in supercomputing.

"If you have a laptop, you probably have four cores, or central processing units, inside your computer," said James Lupo,

Honggao Liu
CCT Deputy Director
Project Principal Investigator

James A. Lupo
CCT Assistant Director of Computational Enablement
Project Director

Image Credit: LSU University Relations

assistant director of computational enablement at CCT and the project director of the SuperMIC project. “The computer is actually sitting there buzzing around on different things simultaneously.”

But for supercomputers made up of hundreds of smaller computers, each with 16 or more processing cores, the task of getting the machine to work on a single problem seamlessly becomes more difficult.

“Now the issue for the programmer is, you have to make those 16 processing cores work on the same problem,” Lupo said.

“It’s like 16 people doing the same task at the same time. But you need some type of coordination to do that,” said Honggao Liu, deputy director of CCT and principal investigator of the project.

Ever since high-performance computing introduced general-purpose graphics cards, or graphical processing units (GPUs), used by the gaming industry to make computers run faster for video games, for example, the burden has increased on programmers to coordinate CPUs and GPUs in the same software applications. Computers that incorporate both traditional processors and graphics card for faster computing require users to learn two different ways of programming them to accomplish work such as weather forecasting.

But the complexity doesn’t stop there.

“Not to be outdone, Intel has developed a brand new processor called the Xeon Phi,” Lupo said. “This now looks like 61 smaller machines, or cores, all put on one card, on one big chip. And plugging one of those into a computer is like adding a baby computer to a bigger computer, because it’s completely separate.”

The new Xeon Phi card, or baby computer, also requires its own programming model.

“Then, if you are really crazy, you put together a machine that’s got a GPU, a Xeon Phi, and the traditional processing units like those inside your laptop, and try to make them all play nice together,” Lupo said.

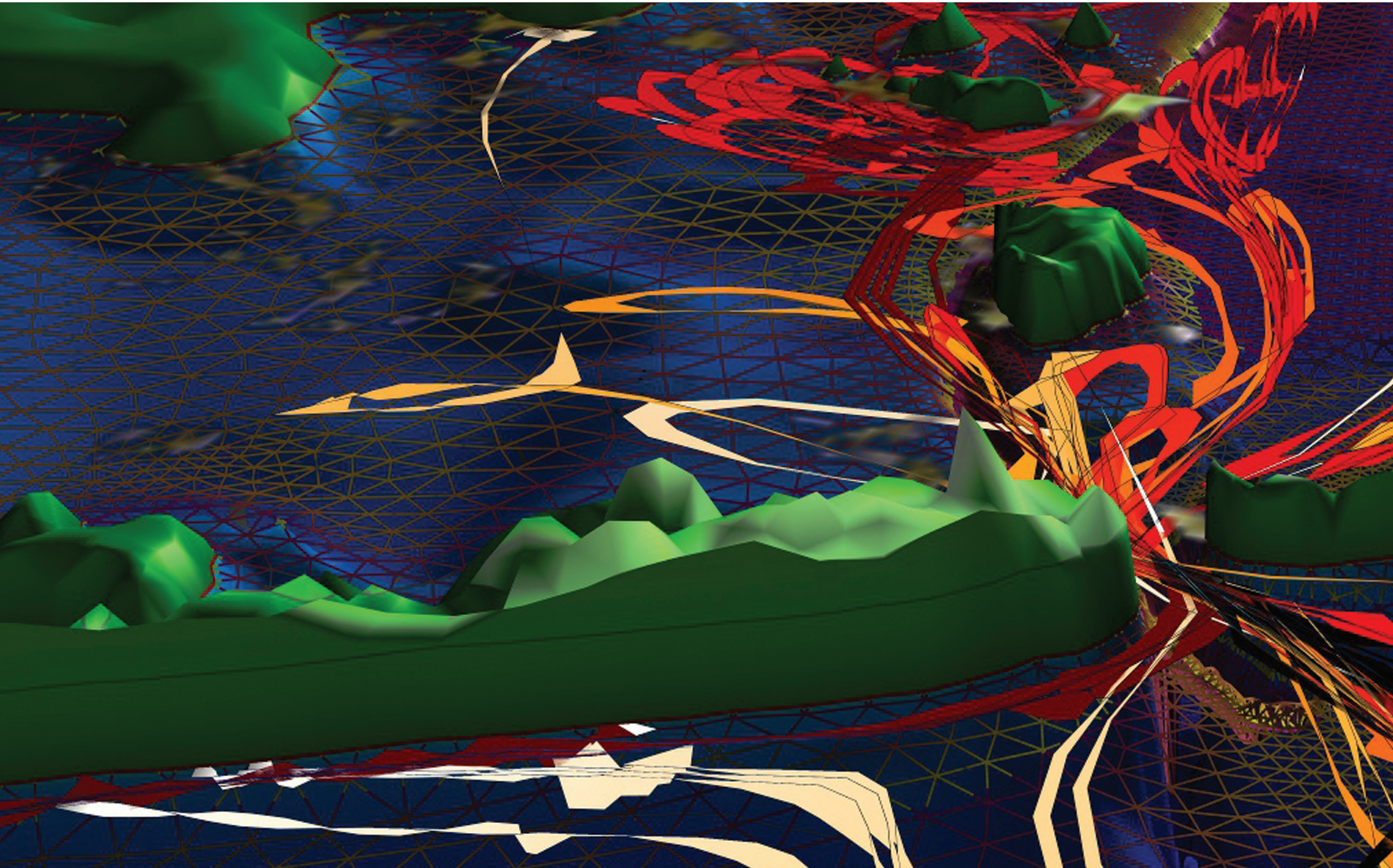
“The new SuperMIC is going to primarily concentrate on Xeon Phi, but some of the servers will have GPU units in them as well, so that our people can really work on cutting-edge applications.”

The total computing capacity, or processing speed, of SuperMIC will be over 1 Petaflops, equivalent to the ability of a computer to do one quadrillion calculations per second. For comparison, the fastest supercomputer in the United States today (the world’s number two system), Titan at the Oak Ridge National Laboratory, is capable of 27 Petaflops.

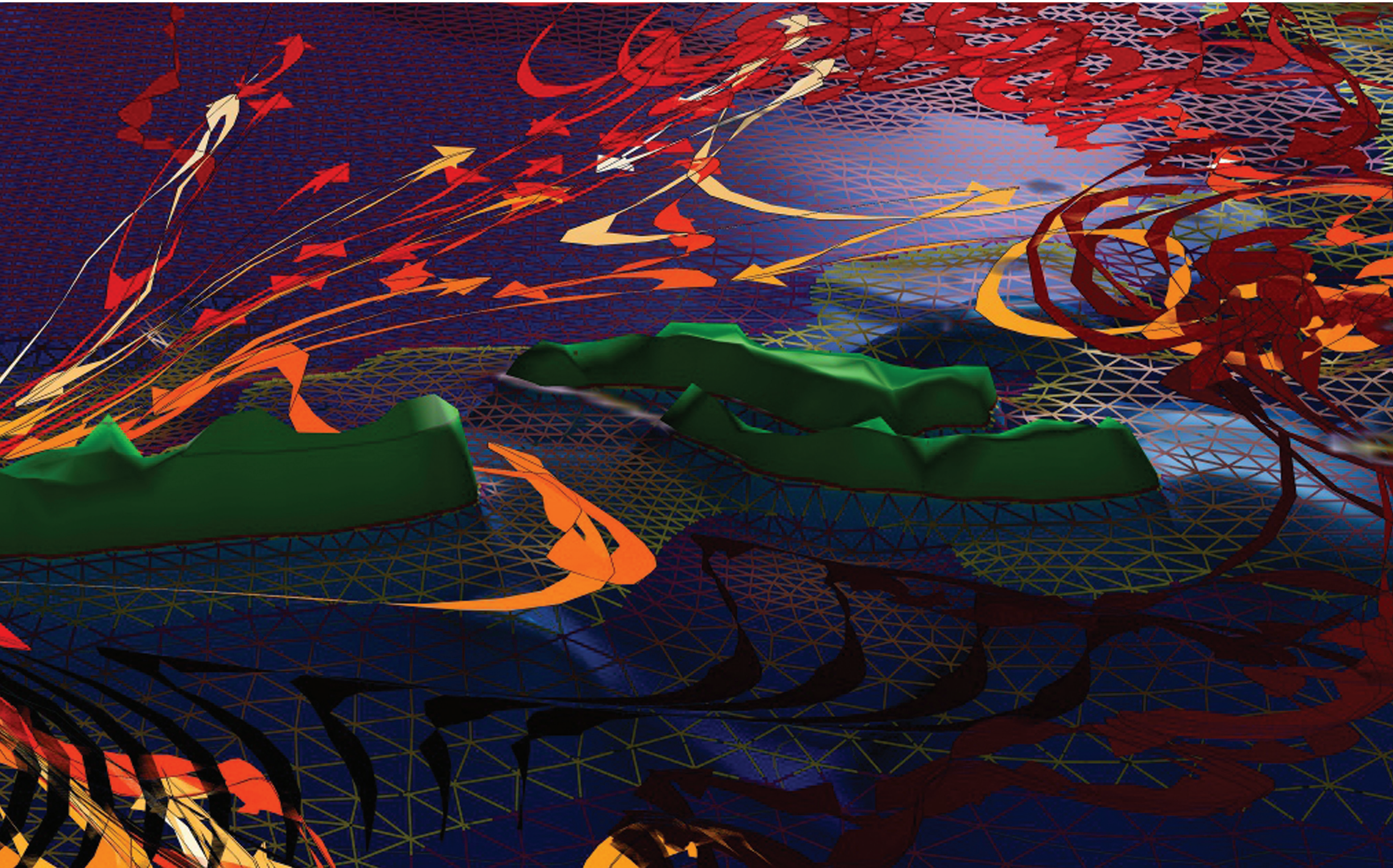
“The future will be for people to use machines that incorporate accelerators such as the GPU and the Xeon Phi,” Liu said. “We are thinking that even the number one supercomputer today could be the new smartphone in 20 years. Right now, developing software for these machines is a burden for the developer, so people really need to learn how to do that.”

So that is the goal with SuperMIC, to train the next generation of researchers to use this type of new architecture, and to help students today learn the skills to program the smartphones and laptops of the future. ◆

ENABLEMENT STAFF



Simulated trajectories of BP oil spill particles in the Barataria Bay south of New Orleans, Louisiana. By CCT IT Consultant and Research Scientist Werner Benger and his graduate assistants, Neha Manya and Isaac Ayyala.



WE VISUALIZE THE FLOW OF BP DEEPWATER HORIZON OIL SOUTH OF NEW ORLEANS

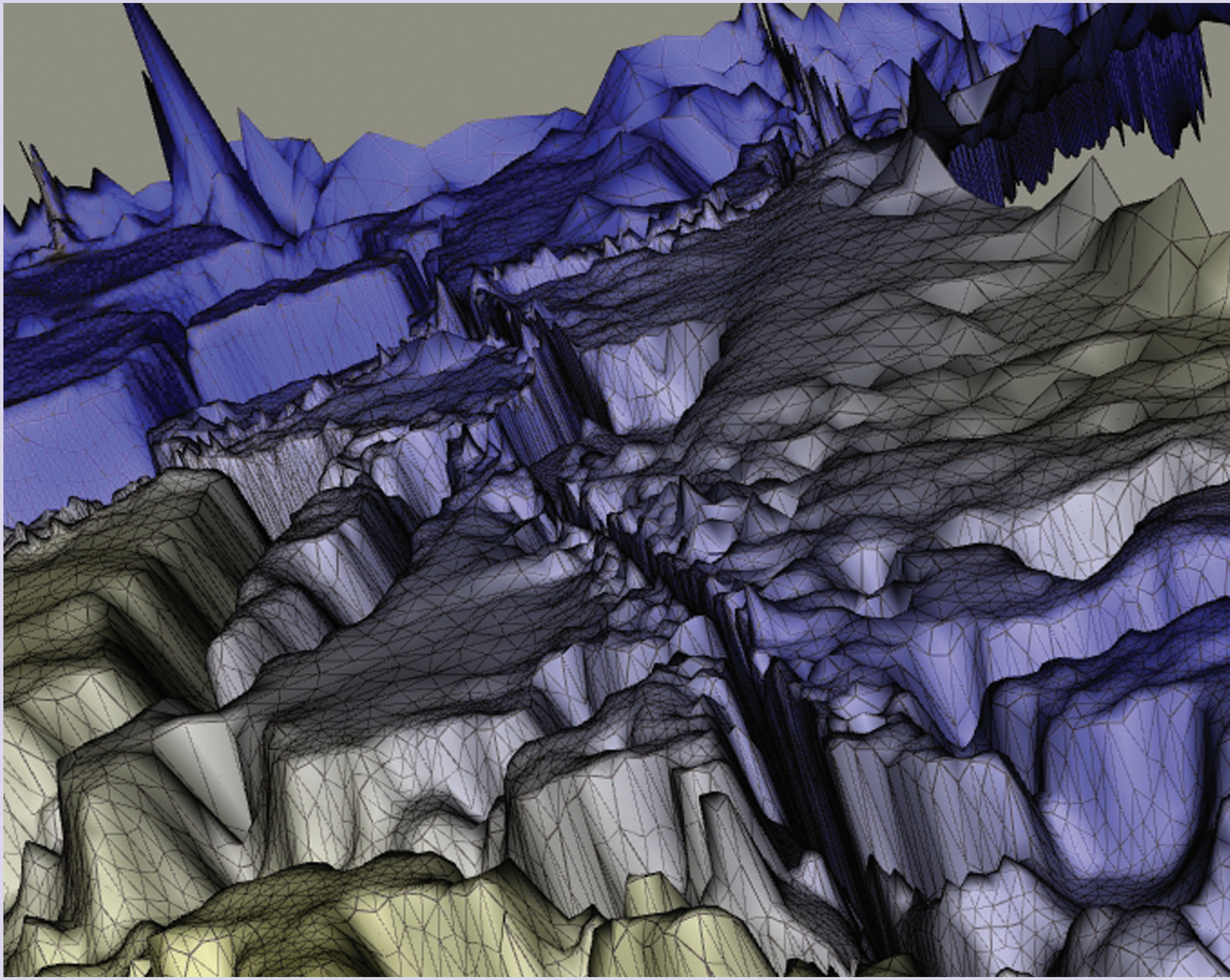
By Tatiana Johnson

Werner Benger knows the importance of a good picture and uses his expertise in supercomputers to accurately visualize complex issues. As an IT consultant and research scientist at CCT, he has been working on a project titled Observations and Modeling to Advance a Louisiana Coastal Circulation and Oil Spill Prediction System since fall 2012.

The project's objective is to investigate the fate of oil particles along the Louisiana Gulf Coast originating from the BP Deepwater Horizon oil spill in 2010. Funding came from BP through grants to LSU and the Coastal Waters Consortium as part of the BP Gulf Research Initiative.

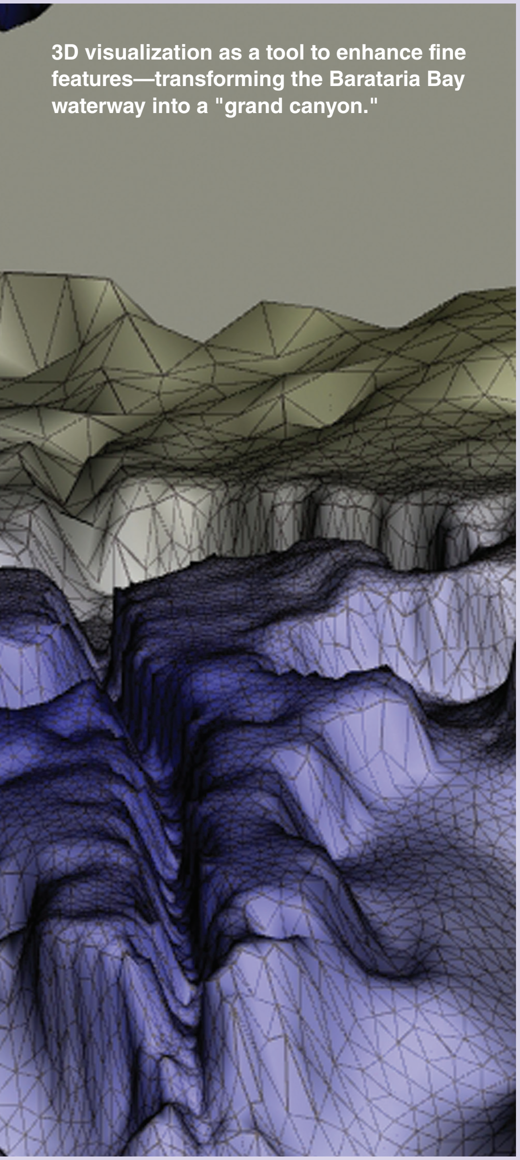
Benger's specific area of interest is Barataria Bay south of New Orleans, a complex estuary connected to the Gulf of Mexico through four tidal passes. It contains several large lakes and numerous marshes interconnected by ponds and channels.

The project is a collaborative effort and is part of a larger initiative implemented by researchers at LSU Department of Oceanography



Dubravko Justic
Texaco Distinguished Professor
Department of Oceanography &
Coastal Sciences
CCT Adjunct Faculty

Werner Benger
CCT IT Consultant and Research Scientist



3D visualization as a tool to enhance fine features—transforming the Barataria Bay waterway into a "grand canyon."

& Coastal Sciences (DOCS), who are doing computational modeling on different aspects of the 2010 oil spill.

"In simple terms, researchers from DOCS, namely Dubravko Justic, Lixia Wang, Nan Walker, and others, make multiple geoscientific and model simulation data sets available to me, and I develop visualization methods to highlight features in these data sets that often allow us to see more than what was originally expected," Benger said.

"Simulations performed in our project predict that BP oil particles originating in open waters close to the Gulf's coastline flow under tidal influence into the Barataria Bay estuary, and some of them return back into the open water," he added.

The ancient art of cartography is an inspiration to Benger. His method of graphic rendering produces results similar to cartographic map views. This approach uses colors to represent ranges of elevation, known as hypsometric tints, and creates topographic contour lines procedurally as part of the rendering process. The use of hypsometric tints is said to have been invented by Leonardo da Vinci in 1503.

To enable the graphic rendering process in 3D, Benger conceived enhancement techniques such as line smoothing, gradient compensation, contour line visibility fading, nonlinear elevation mapping, and shininess variation. All these enhancements were required for a pleasing visual result.

On top of these cartographic data, Benger and his graduate students Neha Manya and Isaac Ayyala can display the oil spill's trajectories. As shown on the image, the particles' trajectories start out in dark red, brighten up to light red, transitioning into orange and yellow as they age. They finish in white colorization at the end of their lifetimes.

"Traditionally, 2D display has been used when working on similar projects," Benger said. "My background is doing 3D and 4D visualization, so I, for the first time, integrated these particular data into a 3D visualization."

As a result, LSU oceanography experts discovered several new features that were not obvious to the research community before.

"Benger's images clearly display prominent features of the estuary such as the Barataria Pass, a tidal inlet that is significantly deeper than any surrounding area," said Dubravko Justic, Texaco Distinguished Professor at DOCS. "It plays a crucial role for the transport of oil in and out of the estuary."

This work was presented at the International Conference in Central Europe on Computer Graphics, Visualization and Computer Vision that took place in the Czech Republic in the summer 2013.

Supercomputers have revolutionized scientific and engineering methodology. They enable researchers to explore theoretical models of phenomena that are either too dangerous, too vast, too tiny, too expensive, or simply impossible for laboratory experimentation. CCT's Werner Benger is at the forefront of bringing scientific visualization into the supercomputing revolution. ◆

WE ENABLE DIGITAL HUMANITIES RESEARCH

Gerald Kennedy
Boyd Professor of English
College of Humanities & Social Sciences

By Tatiana Johnson

As computers become ubiquitous in every aspect of human society, new fields of study emerge. A good example is digital humanities, which combines computing with traditional humanities—history, philosophy, literature, art, archaeology, music, and cultural studies. It applies computational tools in a new domain, using techniques such as data visualization, information retrieval, data mining, statistics, text mining, and publishing.

Since 2011, Chris Branton, IT consultant at CCT and an adjunct professor in LSU's Department of Computer Science & Engineering, has been actively involved in a digital humanities project called Edgar A. Poe, Magazine Editor.

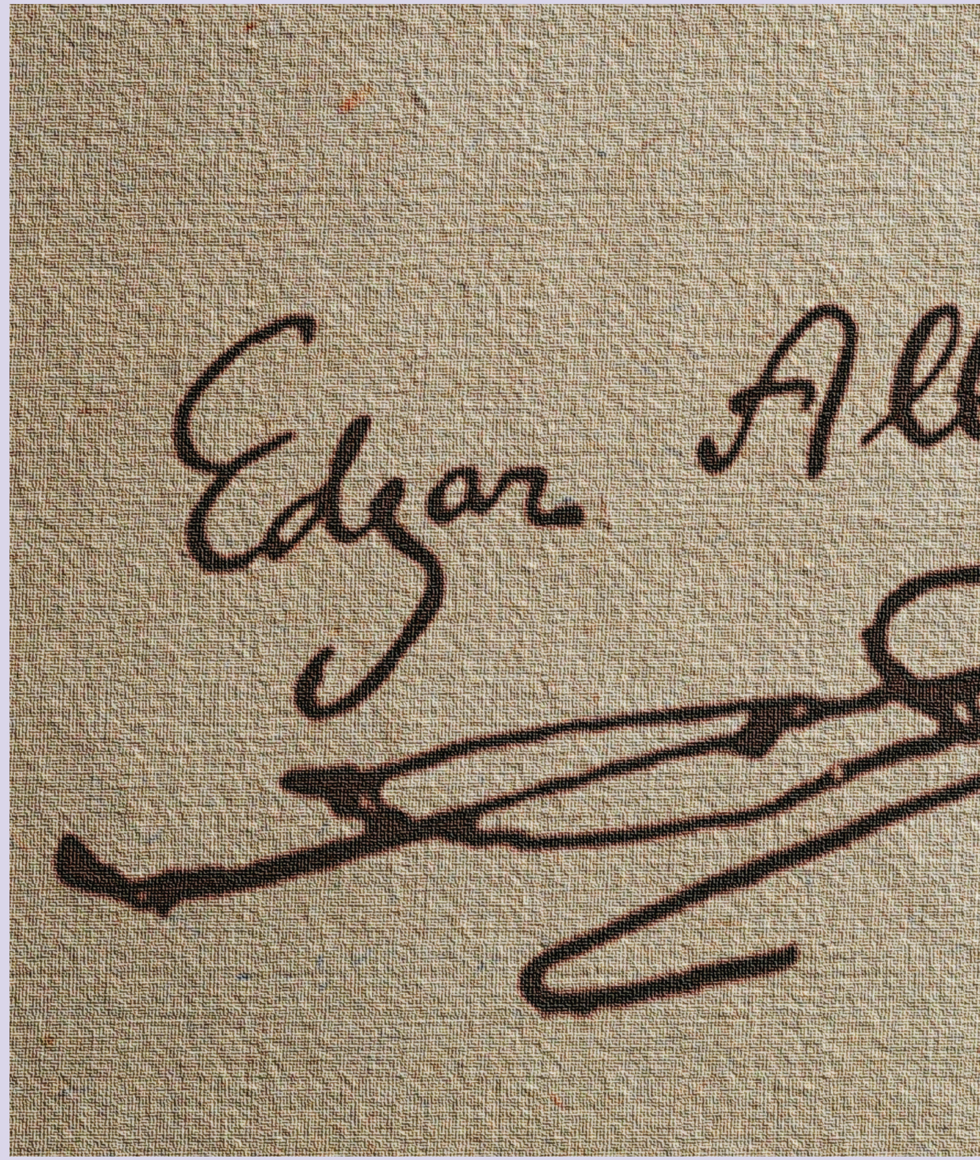
On this initiative, Branton has been providing technological expertise to J. Gerald Kennedy, Boyd Professor of English at LSU, an internationally renowned expert on Poe and the author or editor of seven books about this great American writer.

The idea of a broad antebellum print culture digital resource, built around Poe, was proposed at a Poe symposium in Charlottesville in April 2009, and as co-organizer of the event, Kennedy brought the idea to Baton Rouge. In the fall of 2009, he extended an invitation to faculty in the departments of English, history, computer science, and the School of Library and Information Science to discuss the project.

"When the University's financial crisis slowed work in 2010-11, CCT Director Joel Tohline came to the rescue with funding support that let us hire two graduate assistants and—most instrumental—add Chris Branton to provide sorely needed expertise," Kennedy said.

The project centers around Poe's pivotal role in the print culture of antebellum America. In addition to writing the short stories and poems that have made him an American cultural icon, Poe had great impact as a magazine editor, critic, and proponent of literary culture.

"One thing that fascinates me about this project is how much I learn that is directly applicable to our scientific work at CCT," Branton said. "This may also be a reason that our project has attracted a number of full-time LSU IT employees, including CCT's own Phoenix MacAiodh," he said.

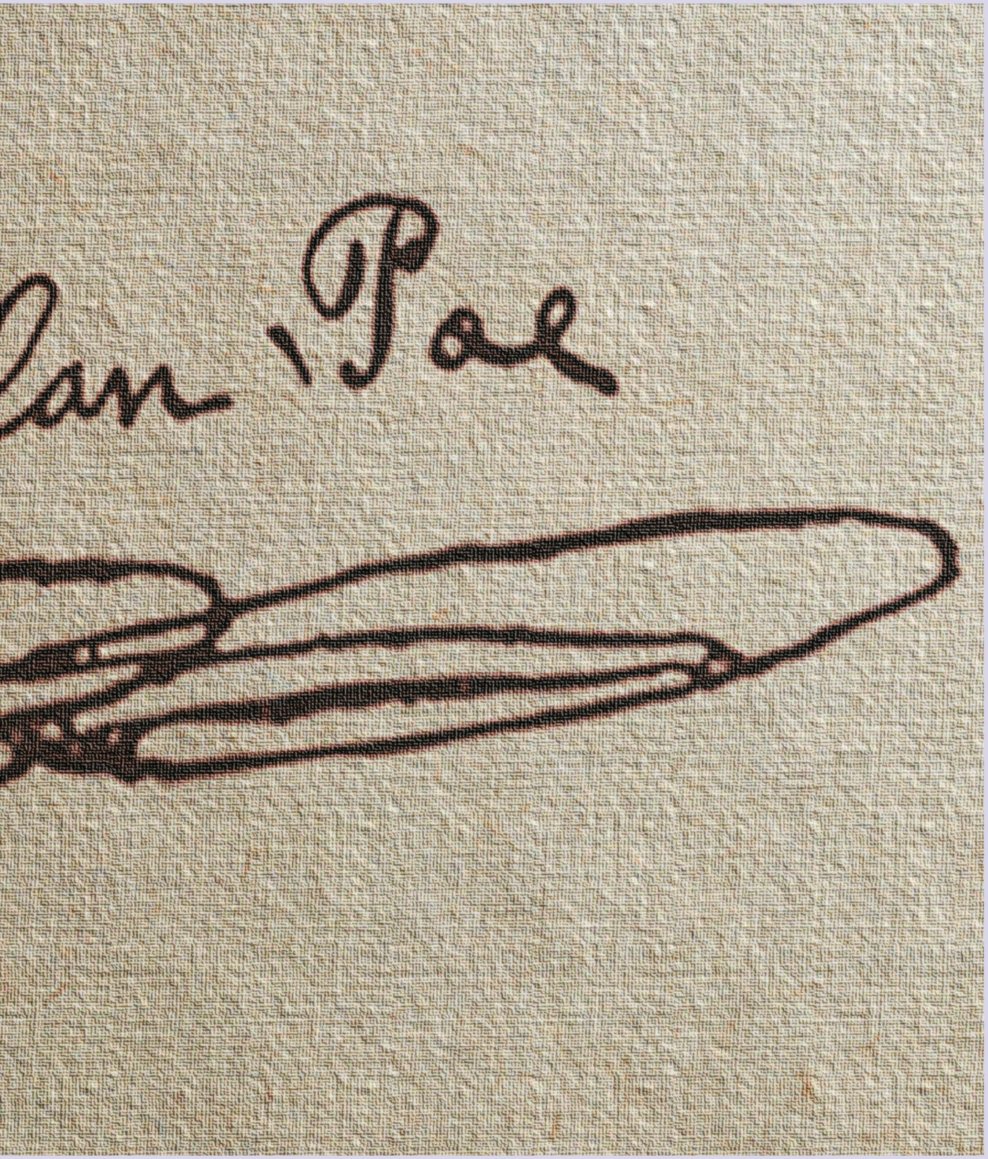


Chris Branton
CCT IT Consultant
Adjunct Professor
Department of Computer Science & Engineering

Derick Ostrenko
School of Art
CCT Cultural Computing Focus Area

Phoenix MacAiodh
CCT IT Analyst & Multimedia Specialist



The aim of the project overall is to allow modern readers to understand more of the cultural and historical context in which Poe's works originally appeared. Like today's films and television series, Poe's work was loaded with references to politics, social movements, and current events. For example, Poe's "The Mystery of Marie Roget," first published in 1842, was based on the actual murder of Mary Rogers in New York the year before. Readers of the time would have made the connection implicitly, while most modern readers would not be aware of the background.

The team's plan is to align paintings, magazine illustrations, political cartoons, and relevant newspaper or magazine articles from the period, and modern graphics (maps and timelines), with reliable, annotated texts of Poe's works. An analysis of topical references in these writings will direct research into the newspapers and magazines likely available to Poe in Philadelphia and New York during these years. This phase of the project is expected to last three years.

How does this multidisciplinary team function? The work is divided into three overlapping groups: humanities, metadata, and technical. The humanities group analyzes literary texts, identifying cultural connections. The metadata group defines the archive's metadata fields and vocabularies. The technical group—CCT's Chris Branton and Derick Ostrenko—manages the architecture of the digital resource, locates and procures the tools required, and creates a look and feel for the website.

"The project's website will provide anybody who is interested with comfortable ways to view print artifacts and annotations, visualize information, and interact with both the content of the website, and the work of scholars," Ostrenko said.

Talking about the significance of the digital humanities field as a whole, Kennedy said, "We do not intend to imply that digital representations are more understandable or enjoyable than their physical precursors. Rather, we want to use the unique capabilities of digital resources to put a number of organized resources at the fingertips of readers. We will contribute to new knowledge by bringing to light connections and associations taken for granted at the time, but mostly forgotten today." ◆

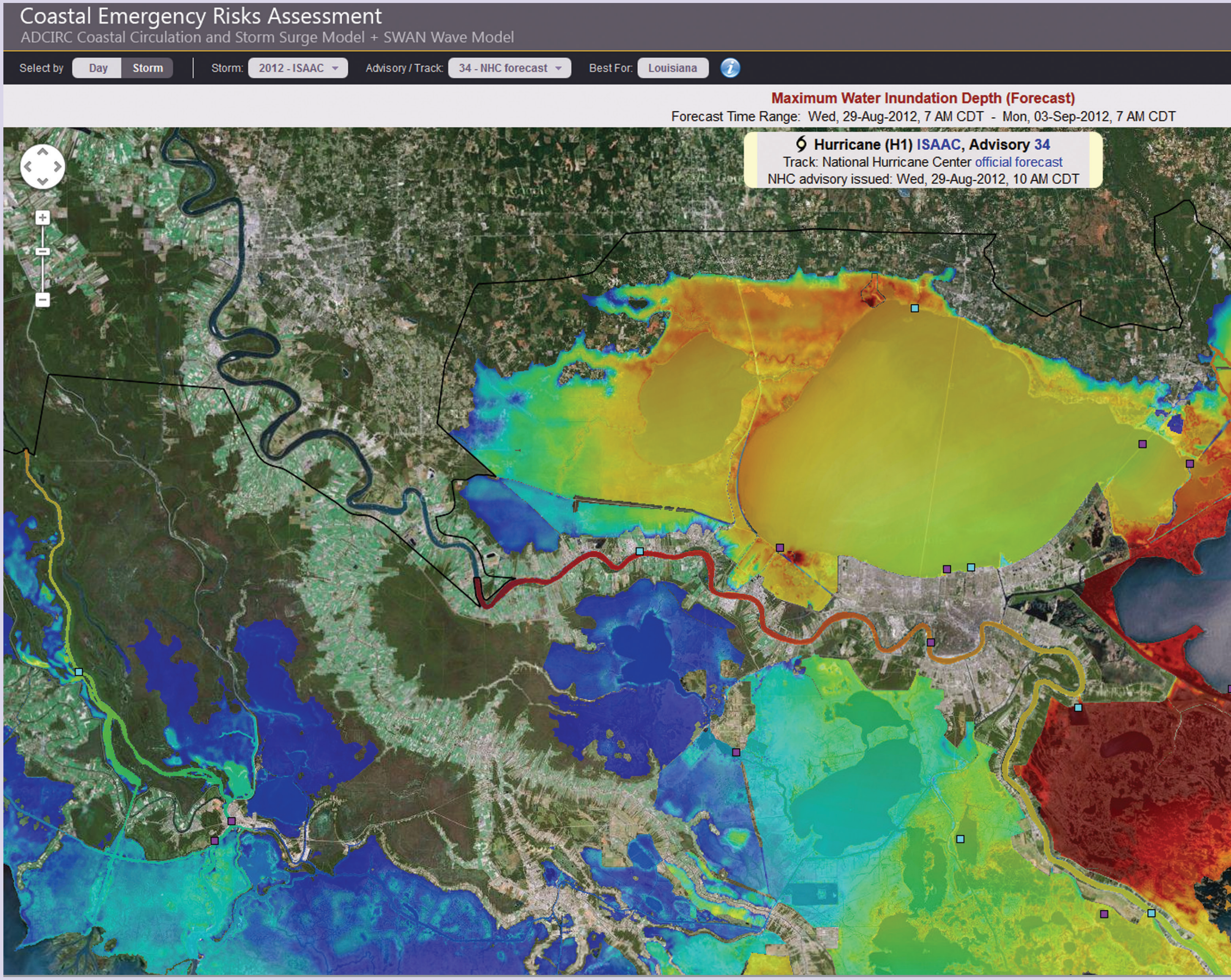
WE SUPPORT LSU'S COASTAL EMERGENCY RISKS ASSESSMENT INTERACTIVE WEBSITE SYSTEM

By Tatiana Johnson

The 2013 Atlantic Hurricane Season began June 1, but Louisiana State University was ready for it. Supported by CCT, scientists at the LSU School of the Coast & Environment developed the Coastal Emergency Risks Assessment interactive website system (CERA). It visualizes several parameters from the ADCIRC Coastal Circulation and Storm Surge Model during an active hurricane. These parameters include storm surge, wind speed, water inundation above ground, and others.

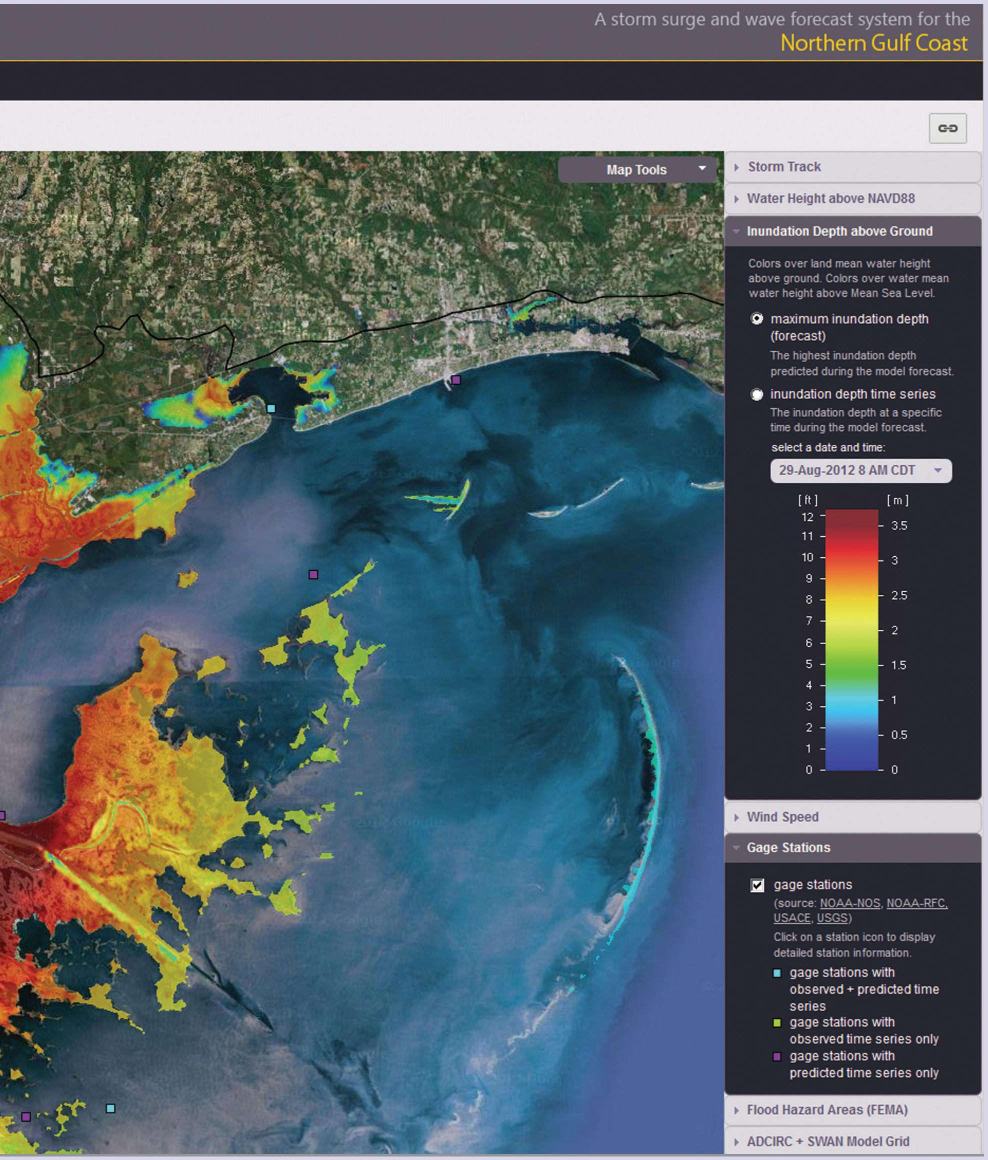
The CERA interactive website system, established with support from Louisiana's Sea Grant and the Coastal Hazards Center of Excellence at the University of North Carolina at Chapel Hill, focuses on two areas—the Gulf of Mexico (http://cera.cct.lsu.edu) and the Atlantic Coast (http://nc-cera.renci.org). The system presents five-day forecasts and delivers the model results every six hours.

"This data can save lives," said Robert Twilley, Louisiana Sea Grant executive director and one of the principal investigators with the CERA project. "It provides emer-



Robert Twilley
Executive Director of Louisiana Sea Grant College Program
Department of Oceanography & Coastal Studies
CCT Adjunct Faculty

Carola Kaiser
CCT IT consultant



gency responders with information on potential hot spots of coastal inundation and suggests where they may need to conduct search anf rescue missions. Planners can look at it to determine where they need to stage relief operations. It also can be used in damage assessments."

The CERA interactive website system is used by the National Hurricane Center, Weather Forecast Centers at the National Oceanic and Atmospheric Administration (NOAA), the United States Coast Guard, and the Governor's Office of Homeland Security and Emergency Preparedness (GOHSEP) in Louisiana.

The model used by the CERA project, the ADCIRC Coastal Circulation and Storm Surge Model, is impressive because of its speed and detail. When Hurricane Katrina made landfall in 2005, computer models used about 300,000 nodes and took four hours to run a storm surge simulation. A node is a unique location on the map where the computer makes physics calculations to determine how water levels will change during a storm. During Hurricane Isaac in 2012, 1.1 million nodes were used on three different storm tracks, and the simulations were completed in two hours using a suite of high-performance computers.

The ADCIRC Coastal Circulation and Storm Surge Model is a multi-facility effort. Partners include Louisiana Sea Grant, LSU, the Louisiana Optical Network Initiative (LONI), the UNC Institute of Marine Sciences, the UNC Renaissance Computing Institute, Seahorse Coastal Consulting, and the ADCIRC Coastal Circulation and Storm Surge Model Group.

"During a hurricane, Louisiana emergency managers meet every morning at GOHSEP, where they discuss the latest and most accurate model results shown on the CERA website," said Carola Kaiser, IT consultant at CCT.

"CCT's specialists insure that all the servers and the network operate smoothly so that results from the model can be delivered quickly, which is the key." ◆

WE DEVELOP CACTUS FRAMEWORK

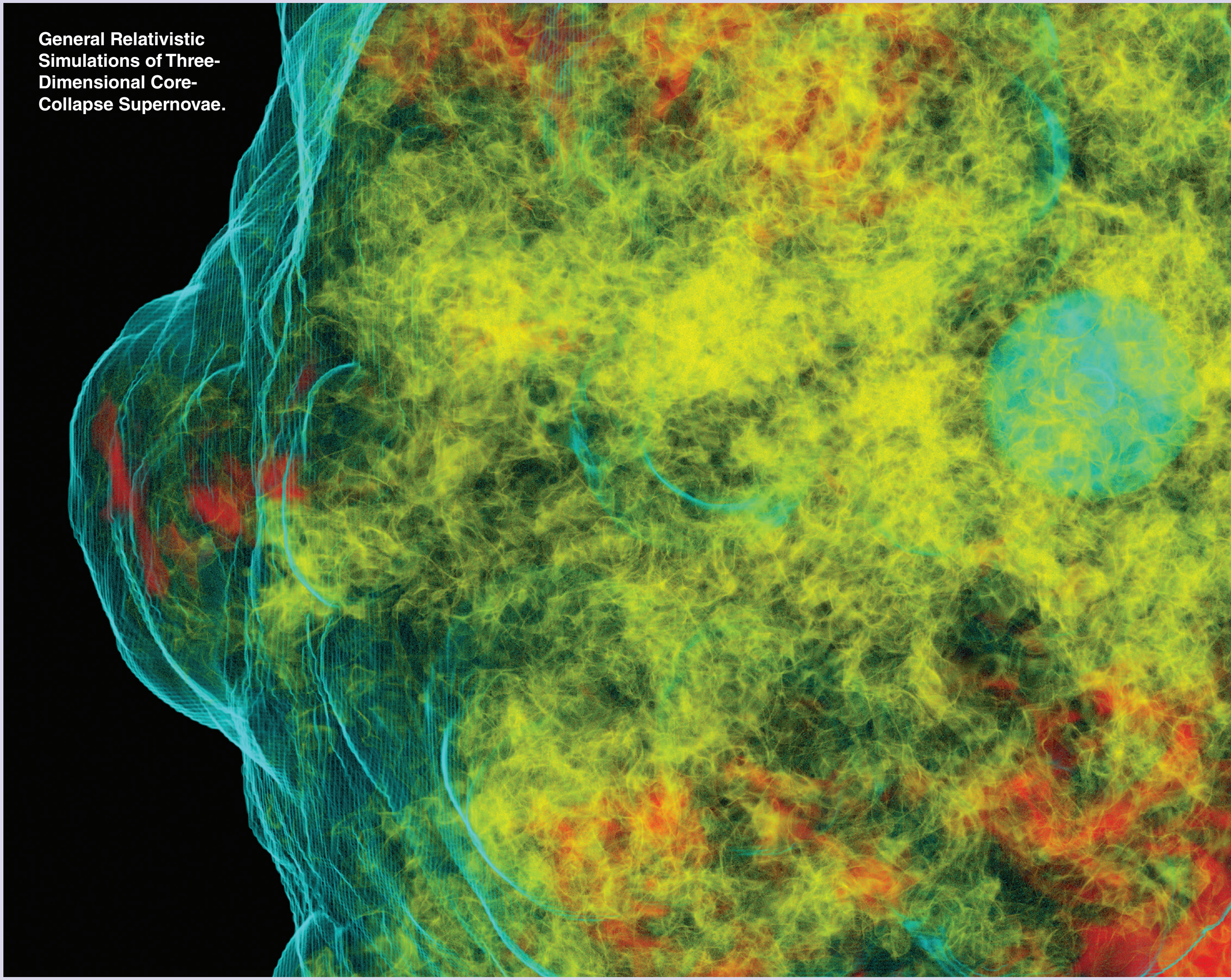
By Steven R. Brandt

The Cactus Framework is an open source, modular, portable, programming environment for collaborative HPC computing. Its abstractions make it easy for its multi-national user community to design and assemble components (both for physics and infrastructure), while relying on Cactus to make these modules inter-operate.

Cactus is used by more than a dozen research groups worldwide to exchange codes and define data formats.

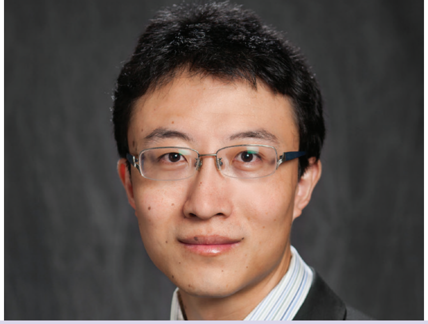
Cactus was originally developed at the Max Planck Institute for Gravitational Physics in Potsdam, Germany, with many contributions from colleagues around the world, including Washington University, Lawrence Berkeley National Laboratory, National Center for Supercomputing Applications, and University of Tübingen.

In 2003, much of the Cactus development moved to the Frameworks research group at the LSU CCT. Researchers in Baton Rouge and Potsdam now work closely together to further enhance and support Cactus.



Steven R. Brandt
Cactus Group Lead
CCT IT Consultant
Adjunct Professor of Computer Science

Frank Löffler
CCT IT Consultant
Cactus Group



Peter Diener
CCT Research Faculty
Cactus Group

Jian Tao
CCT IT Consultant
Research Scientist
Cactus Group

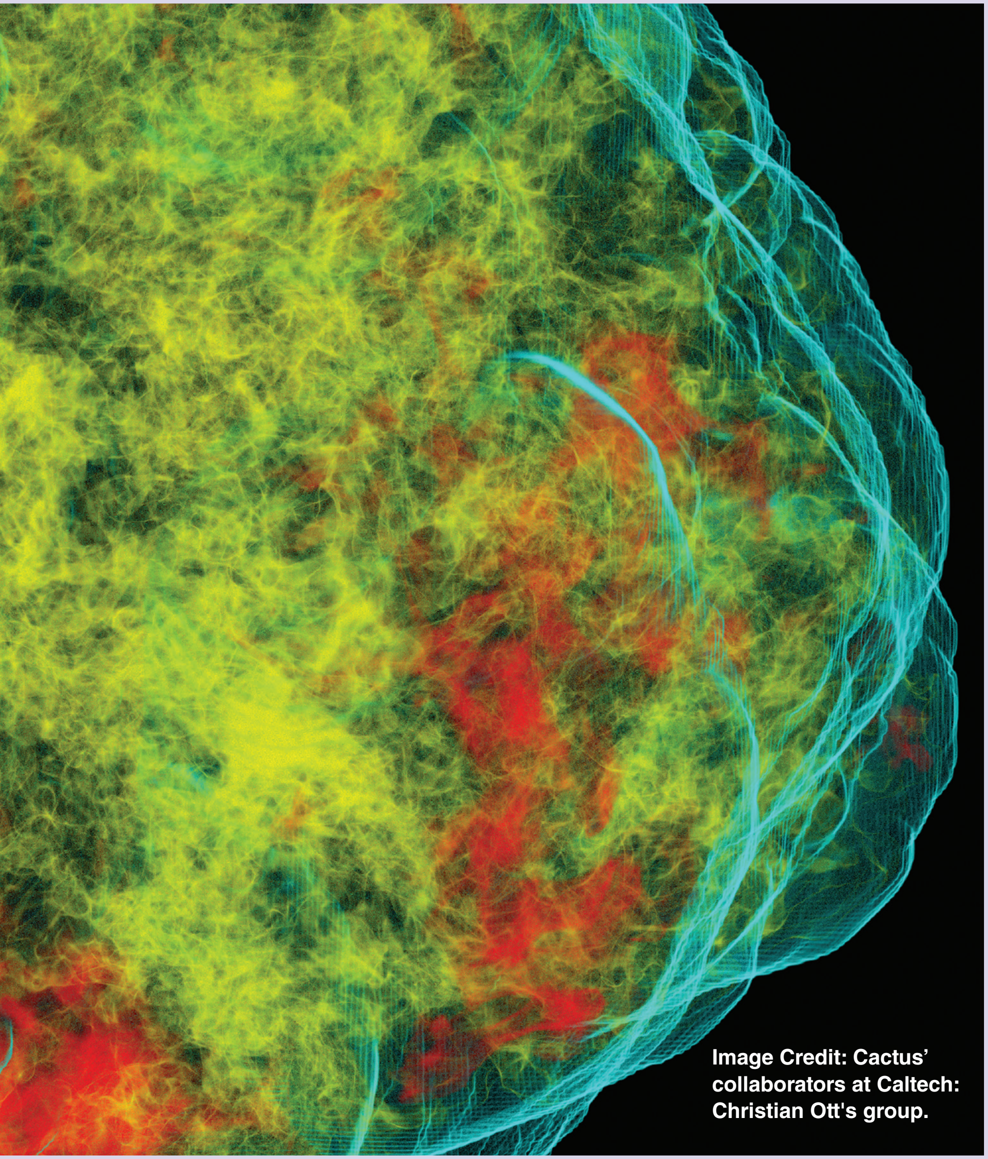


Image Credit: Cactus' collaborators at Caltech: Christian Ott's group.

Cactus contains a generic parallel computational toolkit designed for high-performance computing. This toolkit runs efficiently on platforms of all scales, ranging from personal notebooks to the world's largest supercomputers. It provides parallel drivers, coordinates, boundary conditions, time integrators, elliptic solvers (e.g. PETSc), interpolators, reduction operations, and efficient I/O in different data formats (e.g. HDF5). Generic interfaces are used (e.g. an abstract elliptic solver API) making it possible to develop improved modules that are immediately available to the user community.

Simulation data may be analyzed and visualized by a range of external applications, such as Amira, IDL, or OpenDX, and can also be analyzed in-line by use of a web-server module.

Cactus is used and developed by numerous application communities internationally, including numerical relativity, climate modeling, astrophysics, biological computing, and chemical engineering. It is a driving framework for a number of computing infrastructure projects, particularly in grid computing, such as GridLab, GriKSL, and the Astrophysical Simulation Collaboratory.

The oldest application area of the Cactus framework is numerical relativity. The Einstein equations, which describe how spacetime curves in response to matter, are a set of 10 coupled, nonlinear, partial differential equations. Solving these equations requires large computational resources and advanced numerical methods. One current major goal in numerical relativity is the accurate simulation of two orbiting black holes to determine accurately the gravitational radiation that is produced by such a system.

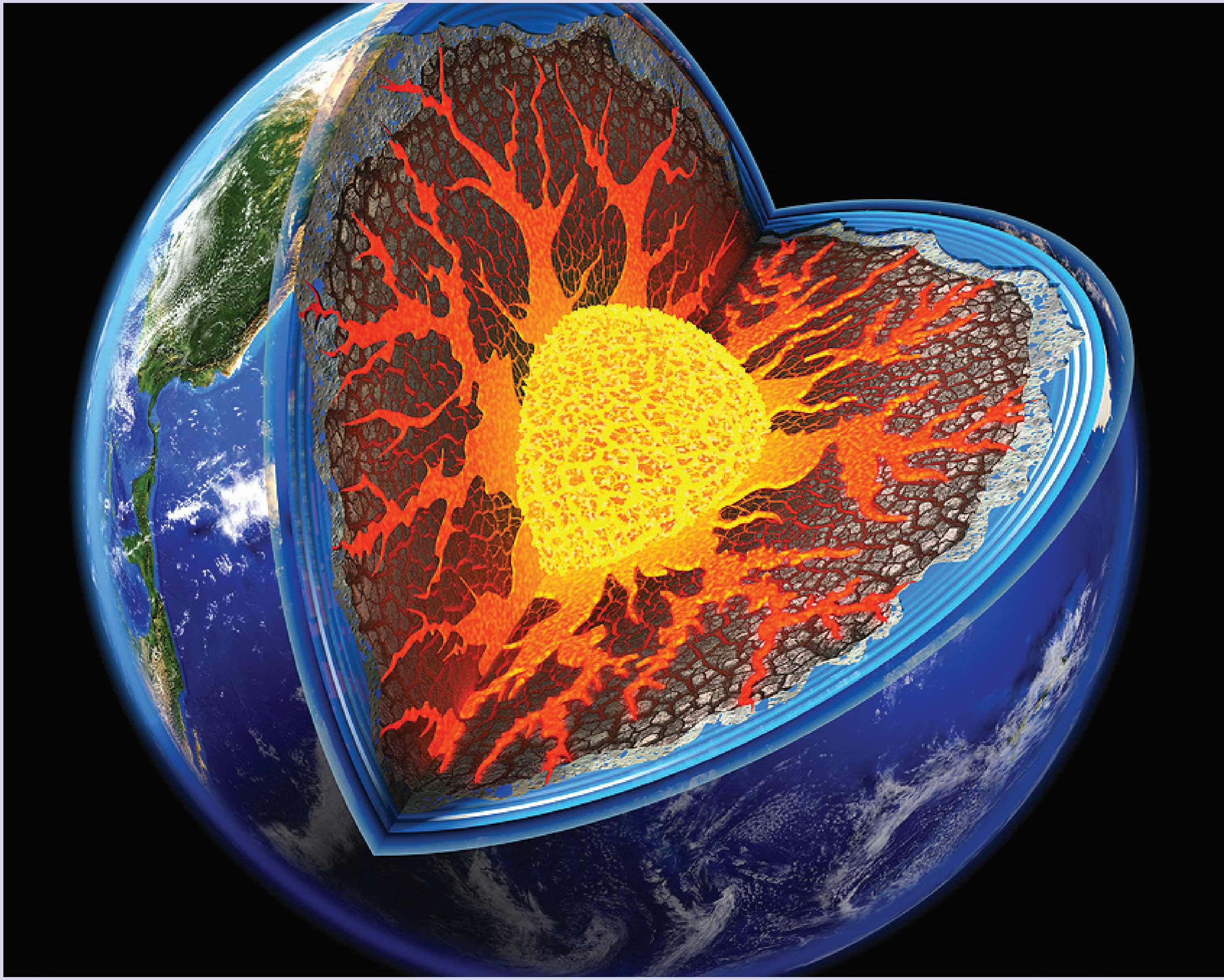
Another major effort at CCT is to establish a computational fluid dynamics (CFD) toolkit within the Cactus framework, which will allow researchers and students to quickly implement their favorite model and experiment with grid topologies, boundary conditions, and solution methods. The scalable multi-processor parallelism that Cactus has to offer will make possible a more interactive approach to CFD. ◆

ECONOMIC DEVELOPMENT


Image Credit: LSU University Relations

WE COLLABORATE WITH CHEVRON TO EXPLORE GEOTHERMAL ENERGY

By Tatiana Johnson



The modern world relies on a vast energy supply to fuel everything from transportation and communication, to security and health delivery systems. As traditional resources deplete, renewable sources become increasingly more important. One of them is geothermal, or the heat of the Earth's core.

Conventional geothermal energy is already widely used today. It relies on finding subterranean reservoirs of heated water where magma comes close to the surface. Enhanced geothermal systems, on the contrary, can harvest energy from hot dry rocks beneath the Earth's surface in artificially created reservoirs. The idea is to generate a network of cracks in the rocks, then inject cold water and let it circulate through the cracked formation. The resulting steam can then be used to produce electricity.

The lack of predictive understanding and numerical simulation of the techniques employed for creating these networks of fractures is what brought Blaise Bourdin, associate professor in the LSU Department of Mathematics and an adjunct faculty

Blaise Bourdin
Department of Mathematics
CCT Adjunct Faculty

Keita Yoshioka
Numerical Geomechanics Consultant
Chevron Energy Technology Company

Christopher White
Department of Petroleum Engineering
CCT Adjunct Faculty

at the LSU Center for Computation & Technology (CCT) to this problem.

In 2008, Bourdin received a National Science Foundation grant, "Applications of Variational Fracture: Enhanced Geothermal Systems" for his research in fracture mechanics.

"Because I am a pragmatic mathematician, I would rather work on a problem that is mathematically challenging and elegant, but also has practical applications. That's what drove me to studying reservoir stimulation."

Bourdin's work is based on the Variational Approach to Fracture. Unlike classical approaches, this method makes no assumptions on where cracks grow and can easily handle interactions between multiple pre-existing and developing cracks.

"We do not need to worry about the direction of the fractures," Bourdin said. "We say, let's just study how they grow. We see that they can merge, split, and do whatever they want in any possible direction, and this is a strength of our approach," he added.

While working on the NSF project, Bourdin met representatives of Chevron who offered to collaborate and extend the original scope of the project, issuing him a grant in 2010. Thus, the academic theoretical research supported by the NSF led to industrial collaboration.

Bourdin serves as the principal investigator (PI) of the project, while the co-PIs are Christopher White and Mayank Tyagi, both faculty in the LSU Department of Petroleum Engineering. Tyagi holds a joint appointment with CCT; White has an adjunct appointment with CCT.

Chevron is one of the world's leading producers of conventional geothermal energy today, and in addition to that, the company is assessing enhanced geothermal systems, studying how energy from hot dry rocks under the Earth's crust can be developed profitably.

"Although we all understand the importance of the fracturing predictability, because of its complex nature, a tractable computational approach is yet to be established in the energy industry," said Keita Yoshioka, numerical geomechanics consultant in Chevron's Houston, TX, office. "Bourdin's project is beginning to shed light in this area."

It turns out the way cracks for geothermal systems are generated is very similar to the way reservoir engineering in the petroleum industry is done, so this research can be applied when drilling for oil and gas.

"The methods Bourdin has developed can model emerging complexities caused by stress fields, fracture interactions, and temperature changes," White said. "This gives us a unique capability to help industry recover more oil and gas economically."

Chukwudi Chukwudozie, a third-year doctoral candidate in petroleum engineering at LSU, is also actively involved on the project. "The easy oils are long gone, so the industry explores and produces from challenging environments," Chukwudozie said. "Companies now need engineers with broad-based skill sets who are capable of interacting with scientists with various backgrounds, which is what I am doing on this project."

There are seven billion people on Earth who use energy each day. Meeting the growing energy demand in a safe and environmentally responsible manner is one of today's key challenges. Currently, numerous organizations within the academic, federal, and commercial sectors conduct research in the field of renewable energy.

"To me, this project is a perfect example of how the CCT enables the collaboration between researchers from multiple disciplines with common interest for computational science, which can lead to rapid technology transfer and industrial applications of theoretical academic research," Bourdin said. ◆

WE INVITE VISUAL EFFECTS COMPANIES TO USE SUPERMIKE-II

By Angela Hartwood

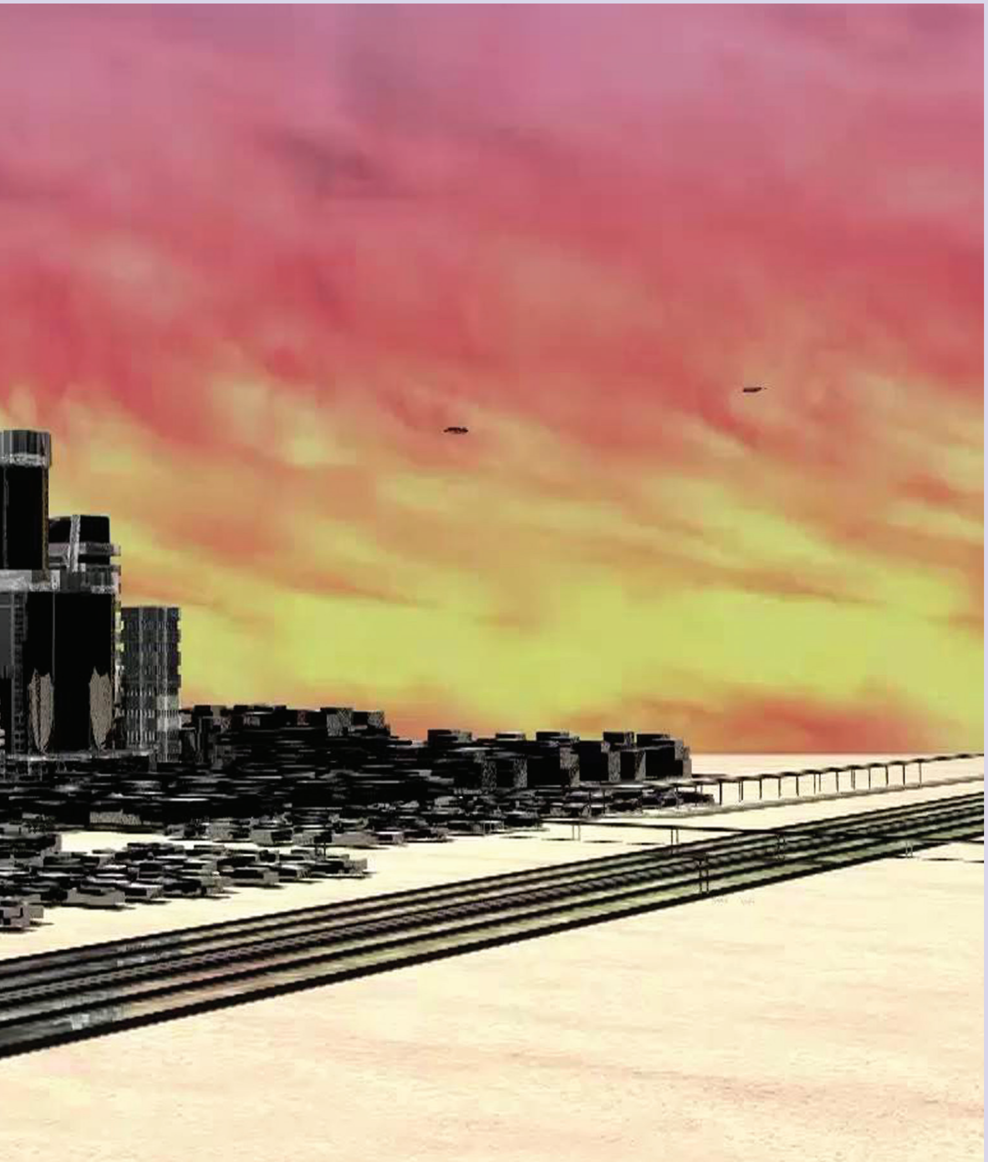
This summer, LSU School of Art students using 3D animation software such as Maya, 3ds Max, After Effects, and CINEMA 4D, were able to offload rendering jobs to SuperMike-II, a 146 TFlops Peak Performance 440 compute node cluster, currently on the top-500 list of the world's most powerful supercomputers. Assistant Professor of Digital Art Derick Ostrenko has been a pioneer in encouraging art students to utilize LSU High Performance Computing (HPC) facilities.

Ostrenko holds a joint appointment at the School of Art and is a member of the Cultural Computing research group at LSU CCT. He was hired as part of the Arts, Visualization, Advanced Technologies and Research (AVATAR) Initiative, in which scholars from across the university are focusing on the intersections between the arts, technology, and computational sciences.

With the help of Marshall Roy, information technology analyst at the College of Art + Design, Ostrenko worked with Lisa Giaime, manager of HPC systems, and Eric Wiggins

Derick Ostrenko
School of Art
CCT Cultural Computing Focus Area

Randy Dannenberg
CCT Assistant Director of Economic Development



and Michael Bryant of CCT to make the render farm accessible to School of Art students.

"Students can render most jobs on their laptops, but this can take a very long time for high quality graphics. By offloading to another rendering source, students can go through numerous iterations without having to wait 20 to 30 minutes between changes," said Ostrenko.

Wiggins and Bryant demonstrated the rendering process in Maya, using a student video of molten lava as an example.

"Working with Derick's students helped us work out the kinks in the rendering process with SuperMike-II," said Giaime. "Finding the sweet spot in the middle of functionality and security was an interesting challenge."

Ostrenko said this resource is a huge plus for students. Besides saving time, students gain experience using an industry-standard pipeline, developing skills that are crucial in the fields of production and animation.

In addition to serving the digital art students, LSU's supercomputing capabilities can benefit local businesses, as well. Until summer 2013, SuperMike-II was mainly used to enable scientific research. In June 2013, however, the LSU Board of Supervisors allowed CCT to offer CPU cycles to commercial entities.

"Companies that wish to offload jobs to SuperMike-II will have the dedicated staff of HPC for support and a render manager capable of working with a multitude of design software," Giaime said.

"Our main mission at LSU is education and research, but we also want to use our technology as an economic development engine in Louisiana," said CCT Assistant Director of Economic Development Randy Dannenberg. "The fact that the art students were able to successfully use SuperMike-II as a render farm shows that we can do it, so we invite visual effects companies to partner with us." ◆

EDUCATION & OUTREACH

Image Credit: Phoenix MacAiodh

WE ENCOURAGE K-12 STUDENTS TO EXPLORE CAREERS IN STEM

By Tatiana Johnson

In the 21st Century technological innovations have become increasingly important as we face the benefits and challenges of a knowledge-based economy. To succeed in this highly technological society, K-12 students are being encouraged to develop greater interest in careers that touch science, technology, engineering, and mathematics (STEM).

"At CCT, we realize the importance of attracting students into the STEM disciplines, and that's why we traditionally sponsor a number of educational opportunities for K-12 students," said Karen Jones, CCT Assistant Director of Outreach.

In 2013, Alice in Computation Land camp was held for the third summer in a row in June, teaching Baton Rouge middle school girls how to create webpages, animation, video games, and movies on the computer.

“The girls seem to be very enthusiastic and open to new ideas,” said Kathy Traxler, camp instructor and CCT education, outreach & training specialist. “We used the Alice 3-D project to tell stories and also built

Karen Jones
CCT Assistant Director of Outreach

Kathy Traxler
CCT Education, Outreach & Training Specialist

Steven R. Brandt
Beowulf Camp's Main Instructor
CCT IT Consultant
Adjunct Professor of Computer Science

Image Credit: Phoenix MacAiodh

games using a project from MIT called Scratch, as well as another project called GameSalad. At the end of the camp, I told the girls they'd been programming all week long, and they were immediately awed that they had written not just one but multiple codes."

“My favorite thing was making my own video game,” said 8th grader Emma Stoecle. “The idea was to shoot apples with the watermelon seeds.”

Before coming to the Alice camp, 7th grader Anne Marie Gahagan did not know that it was possible to make movies on the computer. “My movie was about fish that could talk. The fish were doing tricks and talking to each other. When a person overheard their conversation, he fainted because he was surprised that the fish talked.”

Another educational opportunity, Beowulf Boot Camp, took place in July to raise awareness of supercomputers among high school students and teachers.

Working in small groups, the participants were given a chance to build a Beowulf class supercomputer with their own hands. It is a machine made by connecting several regular computers together into clusters. In addition, participants developed basic applications on the clusters and learned how to carry out simple programming exercises using Python language. The five-day long educational journey culminated with a tour of LSU’s supercomputer SuperMike-II.

“I came to the camp expecting to sit in lectures all day, but it was nothing like that!” said Timothy Holdiness, a high school senior from Monroe, LA, who plans to major in computer science either at LSU or Louisiana Tech.

“I learned how to program in Python and will use this knowledge to make little programs for fun until I go to college and use it for class.”

“I would recommend students going into computer science to think of supercomputers, as a career direction,” said Beowulf camp’s main instructor Steven Brandt. He is a computational scientist at CCT whose background is in using supercomputers to simulate colliding black holes.

“Specialists in supercomputers are in high demand as these machines have become involved with almost every area of life. Even Pringles potato chips were designed using a supercomputer. Diapers currently use a lot of modern technology to simulate how they should work. Supercomputers are everywhere!”

Speaking at the closing ceremony to the camp’s participants and their parents, CCT’s Director Joel Tohline shared his educational background and the technological evolution that took place in his lifetime. An internationally recognized astrophysicist and in all respects a computational scientist, he used a sliding rule to do all calculations in college and purchased his first digital calculator with the money his parents gave him as his graduation gift.

“You are starting out with significantly more advanced technology than what we had,” Tohline said.

“What will you be using 40 years from now? You might have the capability of SuperMike-II in your smart phones, or even imbedded in your brain! I encourage you to take on this adventure and think about what you will use technology for,” he said. ◆

WE HOST STUDENTS FOR A SUMMER OF RESEARCH FUN

By Tatiana Johnson

The 2013 summer was busy for the 16 students who participated in the 10-week Research Experiences for Undergraduates (REU) program at CCT, funded by the National Science Foundation. Coming from a number of different states, some from as far as Massachusetts and California, they were each assigned a mentor and worked hard on cutting-edge research in computational sciences.

CCT is an ideal setting for students to become familiar with interdisciplinary research. Its diverse faculty from many different LSU departments explores areas ranging from coastal modeling, black holes, and materials science to innovative approaches to supercomputing and computational music.

“I dream of a world where personal aircraft reign as cars do now, and I want to be a part of that revolution,” said Yan Li , junior at Cornell University majoring in mechanical and aerospace engineering. “During the 10 weeks here, I hope to integrate the 3D modeling research I’m doing now with a quadcopter project I began at Cornell, so CCT is definitely helping me along

Juana Moreno
REU Principal Investigator
Department of Physics & Astronomy
CCT Material World Focus Area

Mayank Tyagi
REU Co-Principal Investigator
Department of Petroleum Engineering
CCT Coast to Cosmos Focus Area

Peter Diener
REU Mentor
CCT Research Faculty
Department of Physics & Astronomy

there. This experience will help me specify my research interests a little more," Li said.

CCT first hosted 17 REU students in the summer of 2010. The following summer, the program included five REU students and seven RET (Research Experiences for Teachers) teachers supported by the Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA) project.

"I strongly believe faculty need to benefit the community at large," said REU's principal investigator Juana Moreno, who is faculty at CCT and an associate professor in the Department of Physics & Astronomy. "Most people have not been able to access the kind of educational opportunities we have had. For example, my parents could not even complete elementary school. At our program we try to recruit first-generation college students, community college students, and minorities to introduce them to research," Moreno said.

"I recently became interested in biophysics from a research point of view, because it has the potential for many medical and biology applications," said Anya Leach, a senior physics major at West Virginia University. "I hope that my experience at CCT will confirm my chosen career track of staying in academia," Leach said.

"This is my third year as an REU mentor, and essentially what I like is the excitement of the students," said Peter Diener, research faculty at CCT and an assistant research professor in the Department of Physics & Astronomy. "I am trying to give my student a flavor for solving wave equations on computers. I want to build up his skill set to the point where he would be able to write a code to evolve the scalar wave equation on the space time background of a rotating black hole," Diener said.

The final poster presentation took place on August 2. Students shared what they achieved during the summer, and how CCT helped them obtain a valuable research experience that would help them in their future endeavors. ◆

WE INITIATE DIGITAL MEDIA PROGRAMS AT LSU

By Tatiana Johnson

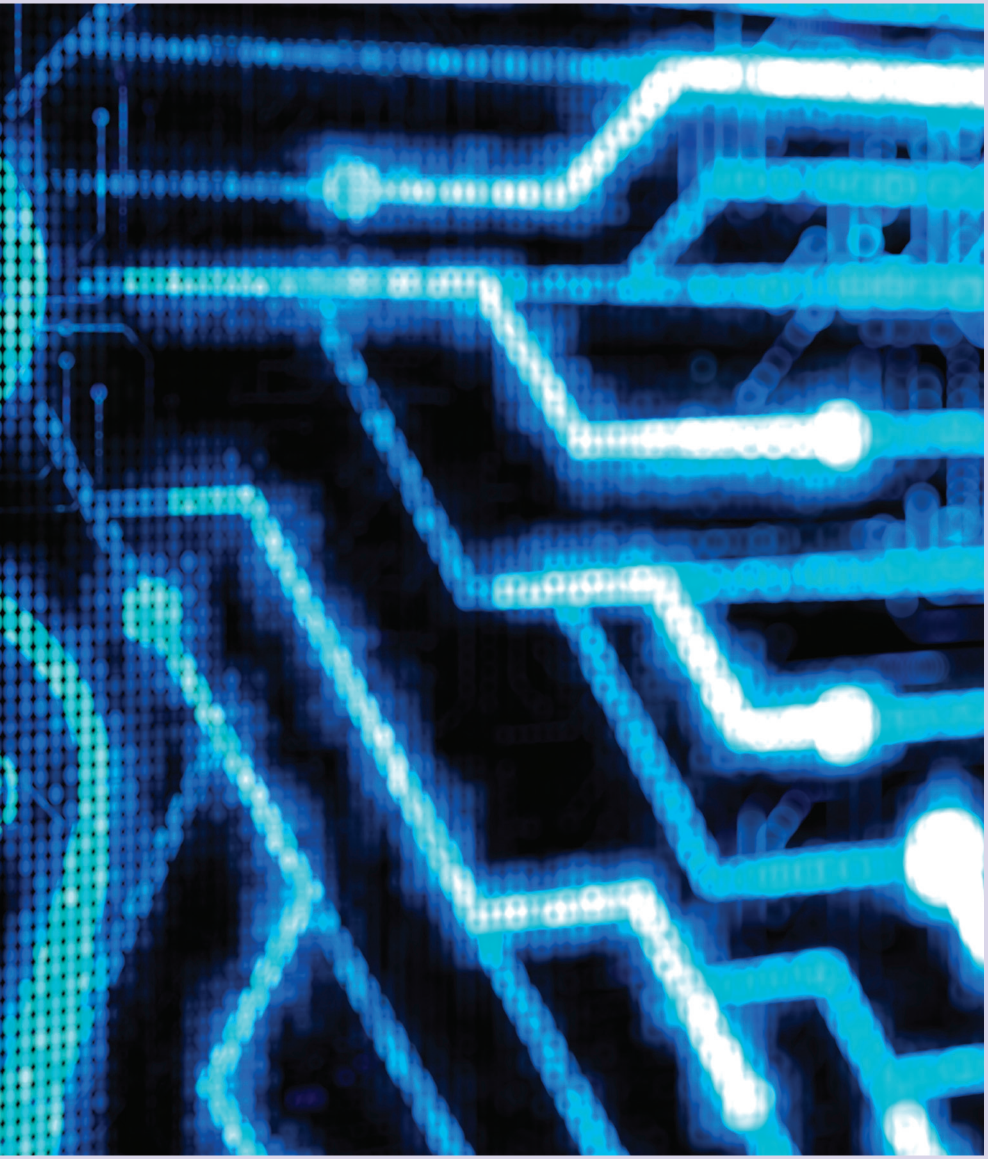
Louisiana is becoming an important player in the digital media industry, which is creating more high-tech jobs. To prepare students for successful careers in this growing industry, in 2010 the CCT's Cultural Computing focus area initiated a digital media minor program at LSU to emphasize the link between arts and technology.

The Cultural Computing group includes 13 faculty engaged in digital media, from LSU units including computer science, electrical and computer engineering, and ISDS/business, to music, art, and mass communications.

One of the courses of this program is video game development. Art students work on animation and character design together with computer science students who primarily program the games.

"I knew I wanted to do modeling for either video games or animation, so as soon as I heard about this course I wanted to see if this was the right path for me," said Margaret Fink, a digital art senior. "I learned a lot about Unity, and, actually, even more about Maya; it's

Marc Aubanel
Director of Digital Media Arts & Engineering Program at LSU



completely different from animation—it blew my mind how different it was."

The course is very unusual in the way it is delivered. Using high-definition video streaming technology, an instructor from LSU teaches in cooperation with a professor at the University of Illinois at Chicago. The students located at either campus can ask questions, providing an exchange that is broader than what a student would get just from a single location.

CCT has been instrumental in the success of this course. In addition to providing all the equipment and the classroom, it has assigned a staff member who is present at each lecture to help with technical issues.

"We are facilitating a couple of major aspects here," said Phoenix MacAiodh, multimedia specialist at CCT. "One, we funded the Planar system, which is the screen that gives such a high-resolution game rendering and stereoscopic capability (3D). We also provide and operate the high-definition streaming technology used to broadcast the course. Before the course starts each January, I make the initial connection and then ensure that everything runs smoothly."

Since 2010, the digital media minor's popularity has prompted the CCT to develop a Digital Media Arts and Engineering (DMAE) master's degree. Marc Aubanel, hired in July 2013 as the DMAE founding director, headed the 500-plus student media arts program at the Art Institute of Vancouver. Among many other accomplishments, he has 14 years of executive-level experience with EA Sports and is founding partner in the original Sanctuary webisodic series.

"The DMAE curriculum will be a boon to businesses in the fields of entertainment, visual effects, video games, television, and animation," Aubanel said.

"One of the key things companies look for when deciding where to establish a business is a talented workforce, and the new digital media master's program will definitely help fulfill the educational component for that industry," said CCT Director Joel Tohline. "We are proud to be contributing to Louisiana's economic development and are looking into the future with confidence." ◆

OUR NEW BUILDING: DIGITAL MEDIA CENTER

By Tatiana Johnson

In August 2013, LSU CCT moved to the brand-new Digital Media Center on South Stadium Drive. The building has several unique capabilities that are still rare in both the academic and private worlds.

“I am unaware of other rooms in North America that have both the Meyer Sound full cinema system, as well as Constellation for musical performance and voice lift in one,” said Bill Schuermann, senior associate design consultant at Houston-based HFP Acoustical Consultants. Since 2010, which was his first exposure to the drawings, Schuermann’s main responsibility has been to envision what technology LSU was going to want when the doors opened in 2013.

According to this technology expert, there are about eight facilities that have a similar system in the United States. Stanford and LSU are the only two universities. University of California at San Diego also has a Constellation system, but it is mostly used for music performance rather than voice lift.

The voice lift Constellation system gives the speaker and the audience the ability to interact better. The theater can seat 206 people, but the presenter can talk without a microphone as if it were a small room.

“You don’t notice the system when it’s on, but you definitely notice it when we turn it off,” said Adam Yates, CCT IT manager.

A commercial theater has standards to adhere to in terms of loud speakers and amplifiers, but the performance of the theater at the DMC is on a totally different level. It is above IMAX, which is considered an advanced system.

There are 82 loud speakers and 26 microphones. The theater meets the SIPTY standards and has 7.1 surround sound capability.

Having a 4K theater is not rare any more. What is different about the DMC theater is that most others have a Sony SRX video projector.

“The Sony projector is what we were going to have here, but I saw the Christie Digital projector at an expo in Las Vegas two years ago and realized it was much better. It makes the picture brighter and sharper,” Schuermann said.

Stephen Beck
Derryl & Helen Haymon Professor of Music
Director, School of Music
CCT Cultural Computing Focus Area

Adam Yates
CCT IT Manager

The building also has a recording studio. The wooden boxes on the walls add reflections, which makes the sound warmer. Opposite those panels is an absorptive panel that prevents echo.

The main contractor, Houston-based HFP Acoustical Consultants, also worked with Coleman Architects and MEP Engineering designing the heating, ventilation, and air-conditioning system.

"They used several tricks, such as applying special materials and running the pipes in a certain way, so the air coming through would not add noise," said Stephen Beck, CCT's Cultural Computing focus area member and director of the School of Music at LSU. "Quiet is very important for making high-quality recordings, and we've never had that type of space anywhere on campus," added Beck.

The individual elements of the theatre are impressive, but equally important is that the new building is a flexible system.

"Take the classroom: you can record, view, see and share information, do video and teleconferencing, add a secondary location, and all these things are network-based and all shared," said Yates.

Steve Ellison, Meyer Sound's applications director for digital products, who is one of the founding fathers of technology upon which Constellation is built, spoke very highly about this building at the annual trade show for the audio/video industry last year.

"Talking about the Constellation voice lift systems his company did in the past year, Ellison gave three examples: in a concert hall in Moscow, Russia, at a military installation in Hawaii, and the third one—at LSU," Schuermann said. "By the way, he spent the most time talking about the one at LSU as it is not just a Constellation voice lift, but also a cinema and a class room," he added.

The platform has been built, and now CCT's faculty, staff, and students will determine how it will be used and how it needs to evolve to meet their needs.

"I will definitely be in touch and will incorporate their suggestions to make the system even better," Schuermann said. ◆

MAJOR ACHIEVEMENTS

Examples of administrative and political decisions made in strong support of the CCT:

- HPC Business Model: The LSU Board of Supervisors approved creation of an administrative revenue account that allows the CCT to sell computing cycles on LSU's HPC systems to private companies. For example, SuperMike-II could be used to support the rendering activities of local visual-effects companies.

- CCT's Status as a Center: Once every five years, the CCT must submit a report summarizing its accomplishments, to date, and requesting authority for continued recognition as a center by the Louisiana Board of Regents. This report was submitted to Academic Affairs in early May, then was approved by Academic Affairs and forwarded to the LSU System Office. On June 7, the LSU Board of Supervisors voted to approve the report.

- Tenure Cases: The Board of Supervisors approved tenure promotions for Mayank Tyagi and Georgios Veronis. Congratulations!

Image Credit: LSU University Relations

Awards and Grants:

- **Hartmut Kaiser, Jeffrey Clayton, Maciej Brodowicz,** and **Juhan Frank** received a $799,682 grant from NSF for five years titled "INSPIRE: STAR: Scalable Toolkit for Transformative Astrophysics Research."

- **Georgios Veronis** received an NSF CAREER award titled "CAREER: Physics-based modeling techniques to enable high-performance nanoplasmonic devices." This is one of the NSF's most prestigious grants, awarded to promising junior faculty who exemplify the role of teacher-scholar through outstanding research, excellence in education, and the integration of research and education.

- **Rudy Hirschheim**, Ourso Family Distinguished Professor of Information Systems and faculty at CCT, was awarded an honorary doctorate by the University of Bern's Faculty of Economic and Social Sciences. The doctorate recognized Hirschheim's pioneering work in the study of outsourcing.

- **Carola Kaiser** received the Department of Homeland Security Science & Technology (DHS S&T) Impact Award for the work with the Coastal Emergency Risks Assessment (CERA) project.

- **Juana Moreno** and **Mayank Tyagi** received a $324,972 grant from NSF for three years titled "REU Site: Interdisciplinary Research Experience in Computational Sciences."

- **Francisco Hung**, Assistant Professor of the LSU Cain Department of Chemical Engineering and CCT received an NSF CAREER award to study the behavior of ionic liquids confined in nanoporous materials. This is one of the NSF's most prestigious grants, awarded to promising junior faculty who exemplify the role of teacher-scholar through outstanding research, excellence in education, and the integration of research and education.

- **Xin Li, Mary Manhein,** and **Warren Waggenspack** received a $447,611 NSF grant titled "RI: CGV: Small: Digital Forensic Facial Reconstruction from Incomplete Datasets."

- **Jorge Pullin,** Professor and Horace Hearne Chair in Theoretical Physics, received a $360,000 NSF grant titled "The dynamics of quantum gravity: symmetry reduced models."

- **Seung-Jong Park, Joel Tohline, Sean Robbins, Lonnie Leger,** and **Gus Kousoulas** received a $947,860 NSF grant for two years titled "CC-NIE Integration: Bridging, Transferring, and Analyzing Big Data over 10Gbps Campus-Wide Software Defined Networks."

- **Honggao Liu, Joel Tohline, Mark Jarrell, Q. Jim Chen**, and **Ram Ramanujam** received a $3,924,181 NSF grant for three years titled "MRI: Acquisition of SuperMIC—A Heterogeneous Computing Environment to Enable Transformation of Computational Research and Education in the State of Louisiana." ◆

NEW HIRES

Marc Aubanel
Digital Media

Hired to lead the new Digital Media master's program at the CCT, Mr. Aubanel previously served as the media arts academic director at the Art Institute of Vancouver. With more than 20 years of experience, including as executive producer at Electronic Arts Canada and a cofounder of a visual effects house, Stage 3 Media, he remains intrigued by his field. "Gaming is still in its infancy compared to other industries, and there are many more incredible breakthroughs to come."

Edgar Berdahl
Music

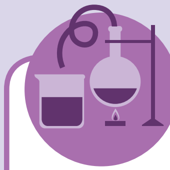
Prior to LSU, Dr. Berdahl served as a postdoctoral fellow at the Technical University of Berlin and a lecturer at the Center for Computer Research in Music and Acoustics at Stanford University where he received his Ph.D in Electrical Engineering. He studies the design of embedded media with a particular focus on making digital interactions seem more "analog." He is the first person to teach designers and artists how to prototype using embedded Linux.

Revati Kumar
Chemistry

Dr. Kumar comes to LSU from the University of Chicago. Her interests lie in the field of material science, specifically in modeling chemical systems that are relevant to the energy storage sector. She was involved in the study of Li-ion transport in rechargeable batteries to understand the structure and dynamics of Li-ion in the electrolyte. Her Ph.D is in theoretical chemistry from the University of Wisconsin-Madison.

Kenneth Lopata
Chemistry

Dr. Lopata's research focuses on plasmon near-field waves and molecule-mediated plasmon transfer. In 2010, he received the first William Wiley Distinguished Postdoctoral Fellowship at the Department of Energy's Environmental Molecular Sciences Laboratory. He received his Ph.D in physical chemistry from UCLA.



William Shelton
Chemical Engineering

Prior to LSU, Dr. Shelton was the Associate Director of the Environmental Molecular Sciences Laboratory at Pacific Northwest National Laboratory, a U.S. Department of Energy government research laboratory in Richland, WA. He received his Ph.D in theoretical condensed matter physics from the University of Cincinnati. The main body of his work is in the general area of disordered systems, alloy theory and surface science where he has worked on incorporating magnetic and chemical disorder including point defects, such as vacancies and antisites in both materials and chemistry.

Cameron Thrash
Biology

Cameron's primary interests are in investigating the biogeochemical roles of microorganisms in marine systems, using a combination of cultivation-based techniques and high-throughput sequencing for a variety of "omics" based approaches. Before joining LSU he had a NSF Postdoctoral Fellowship in Biology researching the genomics and evolution of SAR11 bacterioplankton. His Ph.D. is from UC Berkeley, where his dissertation focused on bioelectrochemical reduction of perchlorate, a major contaminant of groundwater in the United States, isolation of novel perchlorate reducing microorganisms, and side projects involving anaerobic oxidation of iron and uranium.

Jianwei Wang
Geology & Geophysics

Dr. Wang comes from the University of Michigan. His research interests are high performance computer modeling and simulations, applications of quantum chemistry and molecular dynamics in Earth materials. He received a Ph.D. in geochemistry from the University of Illinois at Urbana-Champaign.

R. Clint Whaley
Computer Science

He received his Ph.D from Florida State University in the area of optimizing compilers, and worked at the University of Texas at San Antonio. His research interests include empirical optimization, optimizing compilers, high performance computing, computer architecture and parallel computing.

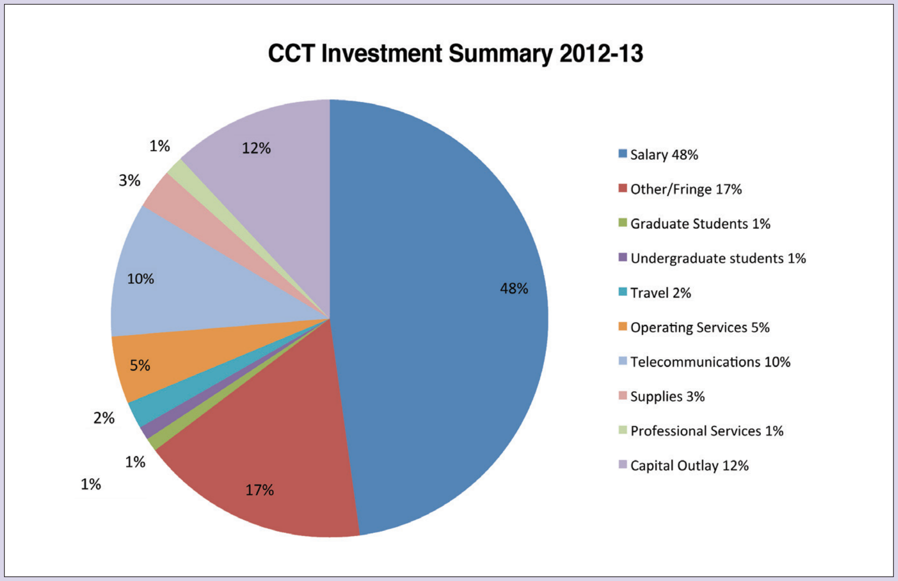
Mark Wilde
Physics

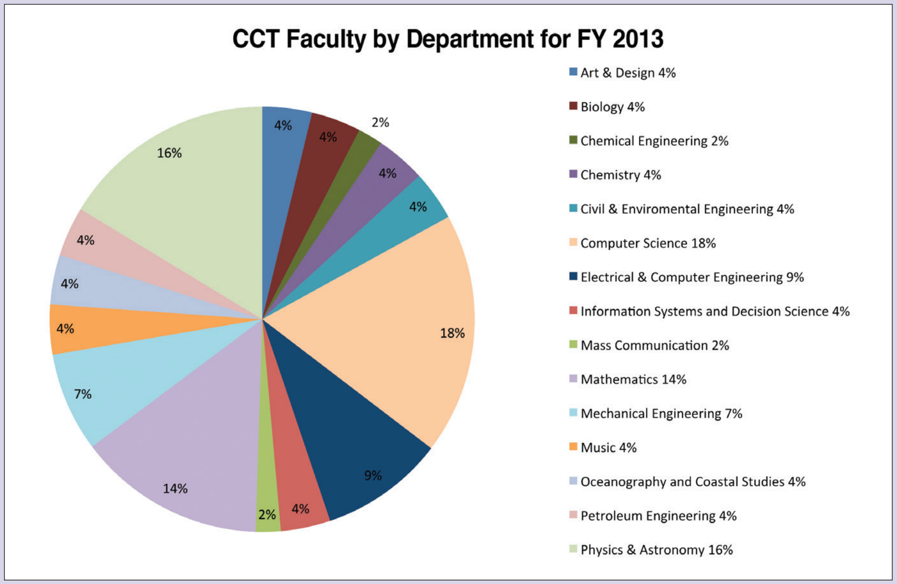
Before LSU, Dr. Wilde worked at McGill University in Canada. His research interests are in quantum information theory, quantum error correction, quantum computational complexity theory and quantum optics with applications to quantum communication. He is the author of *Quantum Information Theory* published by Cambridge University Press. He received his Ph.D in electrical engineering from the University of Southern California, Los Angeles.

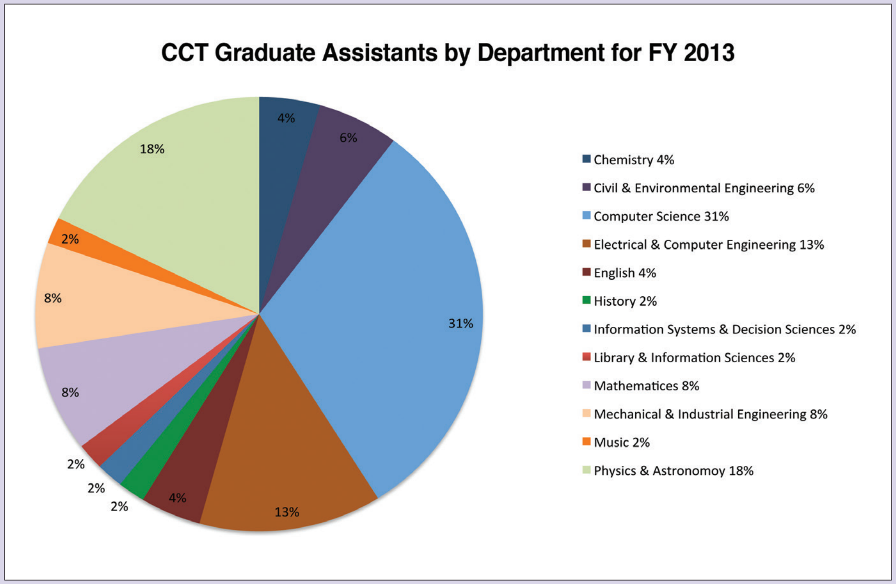
Hye Yeon Nam
Art

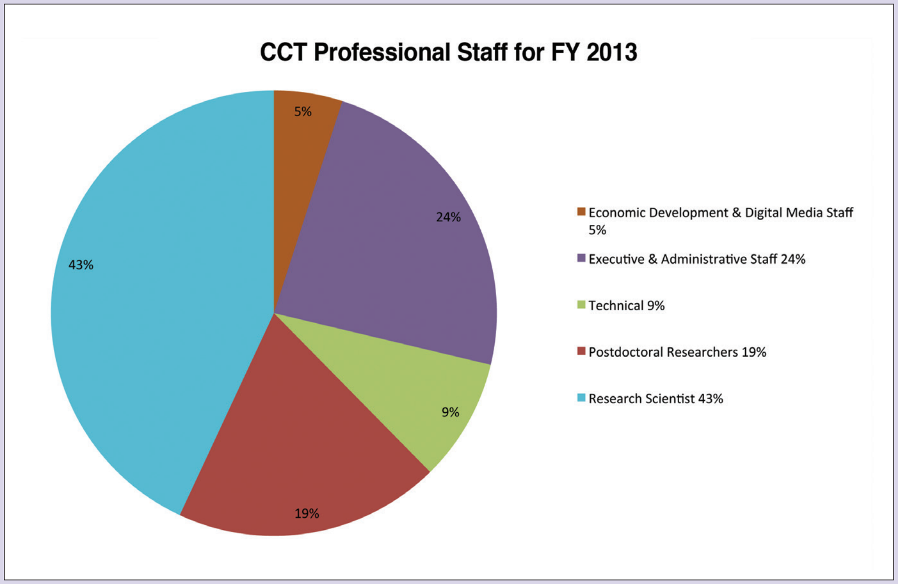
Dr. Nam is a digital media artist working on interactive installations, performance videos, speculative design and experimental games. Her interactive installations are an excellent example of how art and digital media can come together seamlessly to create compelling works of art.

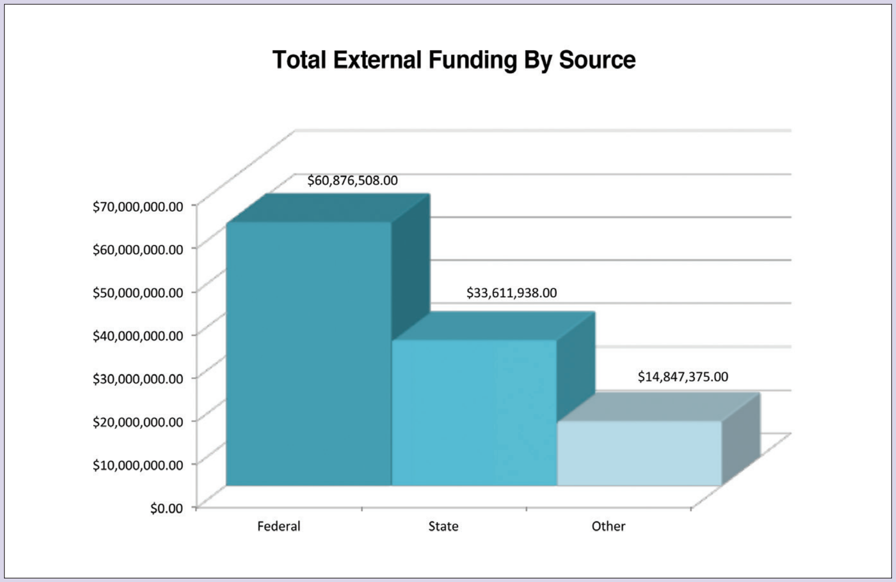
GRAPHS

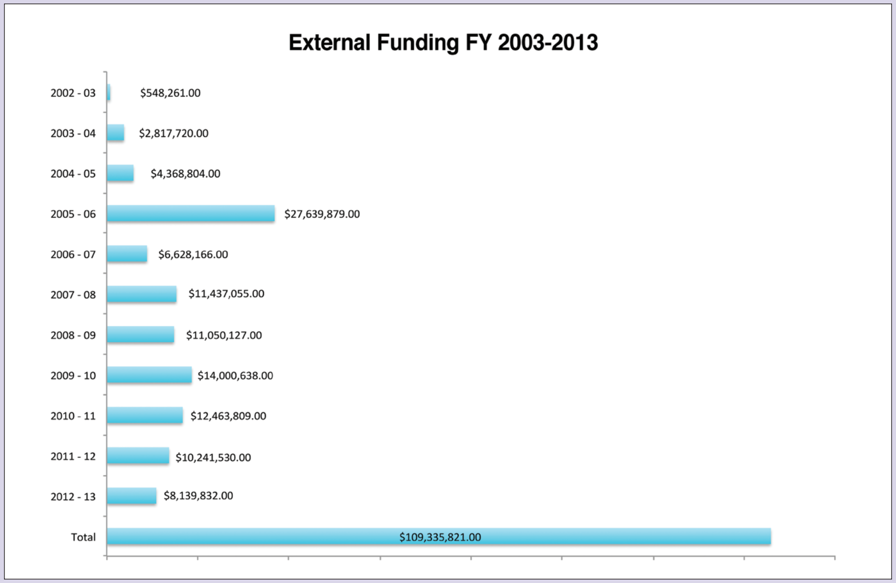

CCT Investment Summary 2012-13
48%
17%
12%
10%
5%
3%
2%
1%
1%
1%
Salary 48%
Other/Fringe 17%
Graduate Students 1%
Undergraduate students 1%
Travel 2%
Operating Services 5%
Telecommunications 10%
Supplies 3%
Professional Services 1%
Capital Outlay 12%


CCT Faculty by Department for FY 2013
Art & Design 4%
Biology 4%
Chemical Engineering 2%
Chemistry 4%
Civil & Enviromental Engineering 4%
Computer Science 18%
Electrical & Computer Engineering 9%
Information Systems and Decision Science 4%
Mass Communication 2%
Mathematics 14%
Mechanical Engineering 7%
Music 4%
Oceanography and Coastal Studies 4%
Petroleum Engineering 4%
Physics & Astronomy 16%


CCT Graduate Assistants by Department for FY 2013
Chemistry 4%
Civil & Environmental Engineering 6%
Computer Science 31%
Electrical & Computer Engineering 13%
English 4%
History 2%
Information Systems & Decision Sciences 2%
Library & Information Sciences 2%
Mathematices 8%
Mechanical & Industrial Engineering 8%
Music 2%
Physics & Astronomoy 18%


CCT Professional Staff for FY 2013
Economic Development & Digital Media Staff 5%
Executive & Administrative Staff 24%
Technical 9%
Postdoctoral Researchers 19%
Research Scientist 43%





Contributors: Andrew Cox and Theresa Markey

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Interdisciplinary | Innovative | Inventive

The Components
Volume 9

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Contact information:
Digital Media Center
340 East Parker Street
Baton Rouge, LA 70803
225.578.4012
www.cct.lsu.edu
info@cct.lsu.edu
Facebook.com/LSUCCT
@LSUCCT

Project Manager: Tatiana Johnson
tjohnson@cct.lsu.edu

Editor: Debra Waters

Graphic Designer: Brittany Ball

Cover: LSU CCT's visualization expert Werner Benger simulates the fate of BP Deepwater Horizon oil south of New Orleans. This image won the Coalition for Academic Scientific Computation 2014 brochure cover competition.

Love Purple
LIVE GOLD

LSU
Louisiana State University