COMPONENTS

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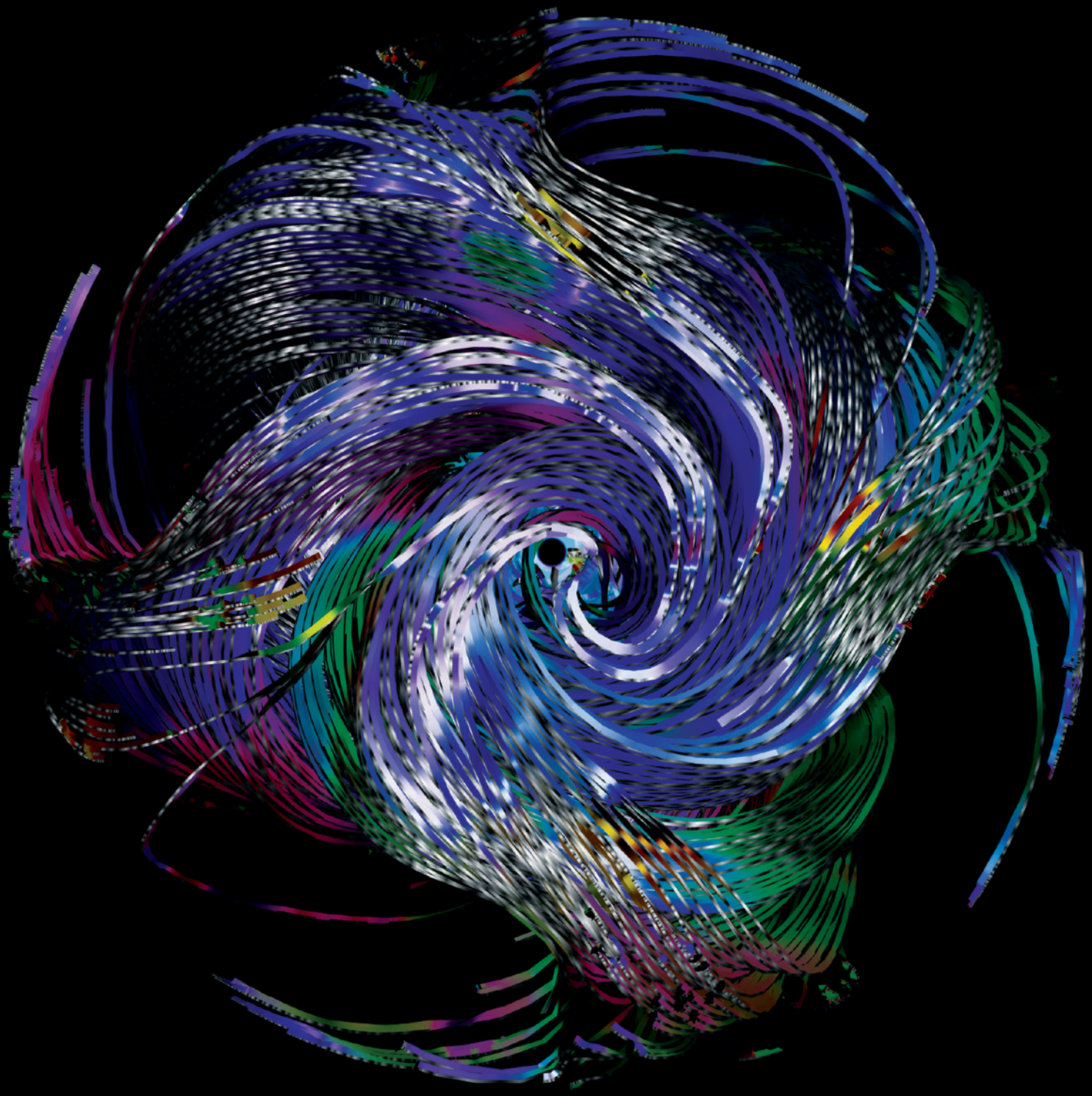


LSU | Center for Computation & Technology

Interdisciplinary | Innovative | Inventive

Contents

Center for Computation & Technology
Louisiana State University
Digital Media Center
340 East Parker Street
Baton Rouge, LA 70803
P: 225.578.4012
F: 225.578.5362
info@cct.lsu.edu
www.cct.lsu.edu
facebook.com/LSUCCT
@LSUCCT

Cover: Visualization of the fluid flow in a stirred tank, showing stream-ribbons emitted from regions of high pressure, depicting curvature and torsion properties within the fluid as mixing indicators, and color-coded by integration parameter. This image is part of a 500 GB simulation dataset. Simulation by Sumanta Acharya and Somnath Roy, Visualization by Werner Benger, Farid Harhad, and Marcel Ritter using the Vish visualization shell.

Components
Volume 10
Components is published annually by Louisiana State University's Center for Computation & Technology (CCT).

CCT is an interdisciplinary research center located on the campus of Louisiana State University in Baton Rouge, Louisiana. CCT advances LSU's Flagship Agenda and promotes economic development for the state by using computational applications to aid research and develop solutions that benefit academia and industry.

CCT is an innovative research environment, advancing computational sciences, technologies, and the disciplines they touch. Researchers at CCT use the advanced cyberinfrastructure – high-speed networks, high-performance computing, advanced data storage and analysis, and hardware and software development – available on campus to enable research in many different fields. By uniting researchers from diverse disciplines, ideas and expertise are disseminated across LSU departments to foster knowledge and invention.

LSU's Vision for Research

Message from the Office of Research & Economic Development

Kalliat T Valsaraj

The Office of Research & Economic Development's significant efforts toward developing a strategic approach to Louisiana State University's research has brought focused attention to areas of current strengths and clarified the vision for the future. As the flagship public university in Louisiana and as a land-grant, sea-grant, and space-grant institution, LSU's mission is to serve the interests of the entire state and the nation. Over the past year, we have made considerable strides in investing in the focal areas identified in our strategic plan and supporting faculty and staff in the ongoing implementation of that plan. One of our major goals is to facilitate more multidisciplinary, cross-campus, and statewide research activities while simultaneously strengthening LSU's existing international partnerships in Asia, South America, and Europe and developing new partnerships. These efforts among other initiatives including increased biomedical and biotechnical research, additional Big Data capabilities, and research in cybersecurity and resilience are just a few examples of our plan for LSU's path to continued success in research and economic development.

LSU's Center for Computation & Technology (CCT) embodies the spirit behind these efforts and is a strong ally in the University's efforts to gain increased prominence on the state, national, and international levels. Supercomputing, high performance computing, and particularly Big Data are key research areas at LSU spearheaded and facilitated by CCT. Partnering with industry giants such as IBM is the perfect complement to our faculty's basic and applied research. We're looking forward to expanding this collaboration to the benefit of our researchers, our students, and our state. I expect CCT will continue to be pivotal in strengthening such partnerships and attracting new ventures. In addition, I expect CCT to play a key role in realizing the goal of LSU 2015 to create a single, globally competitive LSU with statewide reach with enhanced efficiency and productivity in educating its students, creating robust collaborative research, delivering effective health care, impacting economic development, and conducting outreach activities.

I'm proud of CCT's accomplishments and look forward to the new heights this center will most certainly achieve in the near future.

KT Valsaraj, Ph.D.
LSU Vice Chancellor of Research & Economic Development

Message from the Director

I am pleased to bring you the 2014 issue of Components with highlights of the significant contributions of the Center for Computation & Technology (CCT) to LSU, the state, and the nation. These contributions include a variety of ongoing multi-disciplinary research projects; support of undergraduate and graduate education; taking the lead on the development of cyberinfrastructure in support of research; partnership on workforce and economic development initiatives in Louisiana; and continued success in building local, national, and international collaborations. In short, this has been another very good year for CCT.

We have continued to broaden our partnership with LSU's academic units by hiring new faculty members with a keen interest in interdisciplinary collaboration: six new tenure-track/tenured faculty members have come aboard during the 2014-15 academic year, spanning three departments in three different colleges (see page 53). Five of the new faculty hires join LSU's Coastal Hazards Prediction and Mitigation (CHAPM) initiative, a research cluster within CCT, the Department of Civil & Environmental Engineering (CEE) and the Department of Oceanography & Coastal Sciences (DOCS). The sixth faculty member is a joint hire between CCT and LSU's Information Systems and Decision Sciences (ISDS) Department in the E. J. Ourso College of Business. Currently, 34 tenure-track and tenured faculty members at LSU hold joint appointments between the CCT and a home academic department where tenure resides. These appointments span 13 departments in seven separate colleges. I

J. "Ram" Ramanujam

Photo by University Relations

strongly believe that CCT provides a unique environment that promotes convergent research.

During the past year, CCT faculty members have continued to garner significant recognition for their work. Susanne C. Brenner, the Michael F. and Roberta Nesbit McDonald Professor (Math and CCT), was named an LSU Distinguished Research Master; Mark M. Wilde (Physics and CCT) received the National Science Foundation CAREER award; and Hongchao Zhang (Math and CCT) received the LSU Rainmakers Emerging Scholar Award.

At CCT, we have seen continued advancements in research and cyberinfrastructure and supporting LSU's educational mission. Kudos to Hartmut Kaiser for leading the NSF-funded $3 million effort titled "STORM: A Scalable Toolkit for an Open Community Supporting Near Realtime High Resolution Coastal Modeling" (see page 18). Hartmut receives nearly $1 million as the lead PI of this grant, and his collaborators include Joannes Westerink (Notre Dame), Rick Luettich (North Carolina), and Clint Dawson (Texas). The $4 million NSF grant-funded "SuperMIC" supercomputer is now available to high-performance computing (HPC) users at LSU and elsewhere (see page 42). The Digital Media Arts & Engineering master's degree program in collaboration with LSU's College of Engineering, headed by Marc Aubanel, has been approved by the LSU Graduate Council and is being presented to the LSU Board of Supervisors for approval (see page 28). The program is scheduled to admit its first students in the spring of 2015. Also, this issue includes two articles featuring strong ties with industry (see pages 48 and 49). At CCT, we look forward to working closely with the newly established LSU Transformational Technology and Cyber Research Center, headed by Jeff Moulton; we expect this partnership will help diversify and amplify our research and development efforts in applied technology areas.

We bid farewell to Joel Tohline, who after a successful three-year stint as CCT director announced his retirement from the university effective December 2013. Joel had also served as interim director of the center during 2001-2003 when it was called the Louisiana State University's Center for Applied Information Technology and Learning (LSU CAPITAL). We cannot thank Joel enough for all that he has done for CCT and LSU. On a personal note, I have enjoyed his generous and thoughtful mentorship over the years. In addition, we would like to thank Jorge Pullin who served as interim director between January and April this year. Please enjoy the tributes to them in this issue of Components (see page 8).

At CCT, we appreciate the continued tremendous support from the Office of Research & Economic Development at LSU, the university, local, and state leadership. I am thrilled to be leading the Center into the next exciting frontier.

J. "Ram" Ramanujam, Ph.D.
CCT Director

Faculty by Focus Area

Science
Physics
Math
Biology

Engineering
Civil
Chemical
Petroleum
Electrical & Computer
Computer Science

Business
ISIDS

School of Mass Communication

Music & Dramatic Arts
School of Music

College of Art & Design

School of the Coast and Environment
Oceanography & Coastal Sciences

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.

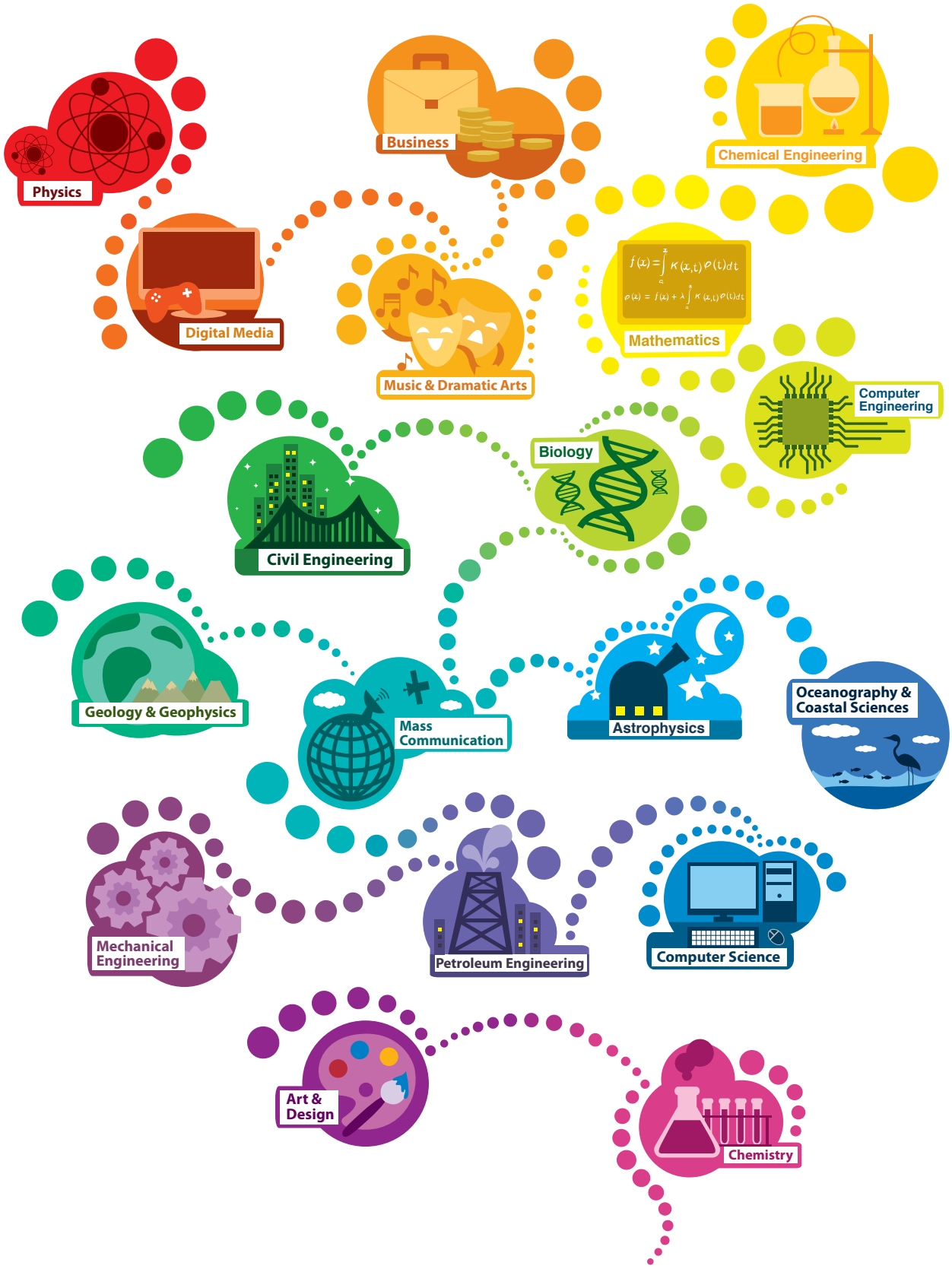
Cultural Computing explores how computational technologies can engage the arts, humanities, and social sciences and how cultural perspectives impact and transform STEM disciplines. Examples include digital art and expression, technology adoption, and interactive computational STEAM.

Core Computational Science 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.

System 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.

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.

Disciplines We Touch



CCT Leadership Transition

Joel Tohline

Tohline Retires

After a successful three-year stint as the Director of the Center for Computation & Technology (CCT), **Joel Tohline** announced his retirement from the university effective December 2013. Tohline also served as interim director of the center from 2001-2003 when it was named Louisiana State University's Center for Applied Information Technology and Learning (LSU CAPITAL). In 2003, as part of the Governor's 2020 Vision Plan, LSU CAPITAL was consolidated and renamed the Center for Computation & Technology.

As director, Tohline was involved in all aspects of CCT, including innovative research in computational science, engineering, and numerous related technologies; ties with Louisiana's promotion and advancement of digital arts and the digital entertainment industry; and educational outreach and training of students K-12, undergraduate and graduate students, post-doctoral scholars, and the general public.

Tohline is a Fellow of the American Association for the Advancement of Science and has authored and co-authored numerous articles in prestigious scientific journals and proceedings on problems related to complex fluid flows in astrophysical systems. Tohline's expertise in utilizing high-performance computers to accurately simulate the processes by which stars form and to simulate catastrophic events that will give rise to bursts of gravitational radiation is recognized worldwide. A total of 18 students earned their Ph.D. under his direction, and he was a lead investigator of grants that brought $9 million in federal and state research funding to LSU.

A Louisiana native, Tohline earned his bachelor's degree in physics from Centenary College in 1974 and his Ph.D. in astronomy from the University of California, Santa Cruz in 1978. Before joining the LSU faculty in 1982, Tohline held a J. Willard Gibbs Instructorship in the Astronomy Department at Yale University and a postdoctoral fellowship in Group T-6 at Los Alamos National Laboratory.

Currently, Tohline is Director Emeritus and Alumni Professor Emeritus of Physics in the Department of Physics & Astronomy at LSU.

Jorge Pullin

Pullin Steps in as Interim Director

After Toline's retirement, **Jorge Pullin**, the Horace Hearne Chair in Theoretical Physics in the Department of Physics and Astronomy at LSU, served as interim director of CCT until May 1, 2014. Pullin's research interests include classical and quantum mechanical gravitational physics, quantum gravity, and black hole collisions.

Pullin attended the University of Cordoba to pursue his Ph.D., which was submitted to and awarded by the Instituto Balseiro, National Commission of Atomic Energy in Bariloche, Argentina, in 1988. He held postdoctoral positions from 1989 until 1991 at Syracuse University and the University of Utah before becoming a faculty member at Penn State in 1993. Pullin came to LSU in 2001.

LSU and CCT are grateful to Pullin for his leadership during the search for the center's current director.

J. "Ram" Ramanujam

Ramanujam Named New Director

In May 2014, LSU appointed **J. "Ram" Ramanujam** as the third director of CCT. Ramanujam was chosen following an extensive international search chaired by LSU math professor and former dean of the College of Arts & Sciences **Guillermo Ferreyra**.

"CCT and LSU have a bright future ahead," Ramanujam said. "I look forward to working with the outstanding administration, faculty, staff and students. Thanks in large part to the current and past leadership at CCT and the enormous support provided by LSU, CCT brings unique research, tools, and infrastructure based on information technology for fostering computation and information-enabled, multi-disciplinary research, and education."

Ramanujam is also the John E. and Beatrice L. Ritter Distinguished Professor in the Division of Electrical & Computer Engineering in the School of Electrical Engineering & Computer Science at LSU. He has been a faculty member at LSU since 1990, has held a joint faculty position at CCT since 2005, and has served as the Systems Science and Engineering focus area lead at CCT since 2011.

He received his bachelor's degree in electrical engineering from the Indian Institute of Technology, Madras in India and his master's and Ph.D. degrees in computer science from The Ohio State University.

Ramanujam's research interests are in compilers and runtime systems for high-performance computing, domain-specific languages and compilers for parallel computing, embedded systems, and energy-aware computing systems. For more than 13 years, he has been a key participant in the National Science Foundation funded Tensor Contraction Engine project involving chemists, physicists, and computer scientists and engineers. He has also played a key role in the Pluto compiler project for automatic parallelization.

RESEARCH

Big Progress on Big Data on Campus

Seung-Jong Park
Photo by University Relations

Huge amounts of data will soon be zipping around campus at jaw-dropping speeds thanks to innovative work being done at the Center for Computation & Technology (CCT). Led by **Seung-Jong Park**, the Big Data Research Integration with Cyberinfrastructure for LSU (BIC-LSU) project is addressing big data challenges and will empower scientific breakthroughs at LSU by providing researchers with advanced information technologies and cyberinfrastructure.

At LSU researchers in genomics, chemistry, coastal science research, and physics are producing big data. The BIC-LSU project will enable their research to be scaled to higher, big data levels with focus on storage, networking, and computing.

As indicated by the name, one of the greatest big data challenges is the size of computer memory requirements

to handle so much data at once. The speed at which big data can be processed is also an important challenge. BIC-LSU is developing software called Parallel Giraph-based Assembler (PGA) that addresses these challenges.

"We're able to provide better performance on time and speed, and we can handle larger data set sizes."

—Seung-Jong Park

"The computation time we're able to achieve with PGA is quite amazing," Park said.

For example, information about a human genome starts with about 500 GB of raw data, which must then be read and assembled into sequence. This process creates about 4 TB of internal data, produces 60 TB of temporal data into hard disks, and takes about 40 hours using current state-of-the-art software.

"PGA is able to do such computations in about 10 hours, or two to three times faster," said Park. "We're able to provide better performance on time and speed, and we can handle larger data set sizes."

The group working on big data at LSU, which includes Park, **Joel Tohline**, **Sean Robbins**, **Lonnie Leger**, **K. Gus Kousoulas**, and other senior LSU faculty, received a $947,860 grant from the National Science Foundation in 2013. Samsung Electronics is an industrial collaborator on the BIC-LSU project.

In part the grant is funding construction of a 10 GB/second speed network at LSU. Labs across campus were connected by fiber optics to the university's supercomputers, which Park calls "a precious resource." By the end of 2014 solid-state drive storage donated by Samsung will have been installed in each lab and integrated into one cyberinfrastructure operated and maintained by BIC-LSU.

Rather than needing their own high-performance computers, LSU researchers will then be able to use a web portal to move 500+ GB of scientific data to be processed and analyzed automatically by the connected computers across campus, and the results of their data computations will be sent back seamlessly.

BIC-LSU is thinking even bigger, looking at challenges for even larger datasets such as those created in meta-genome assembly, or data for about 100,000 species. Working in collaboration with the Joint Genome Institute, a Department of Energy lab, CCT researchers are focusing on ways to handle raw data starting at 1 TB and create more than 40 TB of temporal data.

"In one or two years we expect to be the first to run such huge datasets and do so quickly," Park said.

The team also expects the high-speed network and PGA software to reach beyond LSU's main campus.

"We're concentrating on LSU research first," Park said. "Then we plan to expand the system to other LSU system schools and labs, then across the state and beyond."

See http://bigdata.cct.lsu.edu for more.

Applying Quantum Technologies to Computer Science

As a computer engineering undergraduate at Texas A&M University, **Mark M. Wilde** first read about quantum computers and was blown away by the idea of computers capable of so much more than computers of that time. His life goal became to learn quantum mechanics – the principles on which quantum computers would work. After some years, he began making fundamental contributions that have had a lasting impact on the fields of quantum computation and communication.

Wilde's work eventually led him to the Department of Physics & Astronomy at Louisiana State University, where he is an assistant professor and holds a joint appointment with the Center for Computation & Technology (CCT). Currently, Wilde is working to develop algorithms for quantum information processing that could help make quantum computation and communication a reality.

"One major question that drives my research is to find out what are the fundamental limits of communication," Wilde said. "In order to do so, you need to bring the laws of quantum mechanics into the picture. My work is interdisciplinary. The field of quantum communication draws on physics, mathematics, computer science, and electrical engineering."

The basic building block of a quantum computer is a qubit, just as the bit is for an ordinary computer. A qubit is the smallest quantum system imaginable, and like a computer bit, it has two states: on and off. But, in some sense, qubits can be both on and off at the same time. Along with an odd phenomenon called entanglement, in which quantum particles are very strongly correlated, these simultaneously on-and-off states are responsible for the much faster speeds expected with quantum computing.

"It's also hard to simulate quantum systems with ordinary computers," Wilde said. "For example, there are so many different states of 500 qubits that describing the evolution of them according to quantum mechanics would require a 2^{500} by 2^{500} matrix of numbers. That's hard to do on an ordinary computer."

Building a quantum computer is a very complex challenge, since individual atoms, electrons, or photons must be addressed and managed. In the operation of a quantum computer, a lot of errors can arise when processing finely tuned qubits due to their interaction with the surrounding environment, causing the qubits to lose information. However, quantum error correction algorithms have been devised to avoid the deleterious effects of these environmental interactions, and "they can be simulated using the supercomputing resources at CCT," Wilde said.

A quantum computer, once developed, would be able to crack the encryption codes we use today. This is one major application of quantum computers that has interested corporations such as IBM, Google, and Lockheed Martin, among others, in addition to various governments around the world.

On the other hand, "what quantum takes away it also gives back," Wilde said. "Quantum key distribution would provide stronger security than any current cryptosystem in use because if someone tampers in any way with the transmission of quantum information it could be detected. This is a consequence of the uncertainty principle, a cornerstone of modern physics, and quantum key distribution algorithms are based on this principle."

In a recent *Nature Communications* journal article, Wilde and his coauthors published their findings on quantum secured communication protocols. In particular, their work discusses the limits on secret data exchange over long distances. He and his coauthors proved mathematically that the rate at which information can be communicated securely, even using the laws of quantum mechanics, decays exponentially with the distance over which the data is communicated. More simply, the greater the distance between two quantum computers communicating, the less chance there is that these two quantum computers can communicate securely. However, this loss can be mitigated through the use of a device called a "quantum repeater."

Wilde collaborated on this project with a researcher in Tokyo and a colleague at Raytheon BBN Technologies in Cambridge, Maine. He also has active collaborations with various research groups around the world. Along with **Jonathan P. Dowling** and **Hwang Lee** of the Quantum Science & Technologies Group, Wilde jointly supervises Ph.D. student **Bhaskar Roy Bardhan** who will soon graduate and start a postdoctoral position at MIT.

STE||AR Group Releases HPX v0.9.9

The **Systems Technology, Emergent Parallelism & Algorithm Research** (STE||AR, pronounced stellar) Group at the Center for Computation & Technology (CCT) is proud to announce the release of HPX v0.9.9. This release includes more than 140 bug fixes and 1,300 commits to the codebase. With these changes HPX moves closer to its goals of being a portable, dependable, and easy-to-use runtime system.

The STE||AR Group includes faculty, researchers, and students from around the world who strive to find new and more efficient ways to utilize today's and tomorrow's computers. One of the group's focus areas is on the development of the ParalleX execution model and its implementation in the group's HPX (High Performance ParalleX), an experimental, general purpose C++ runtime system for parallel and distributed applications of any scale.

ParalleX is a new, and still experimental, parallel execution model that aims to overcome the limitations imposed by the current hardware and the way applications are written today. The STE||AR Group focuses on two types of applications – those requiring excellent strong scaling, allowing for a dramatic reduction of execution time for fixed workloads, and those needing the highest level of sustained performance through massive parallelism.

Using conventional practices, these applications are unable to effectively exploit a relatively small number of cores in a multi-core system. More often than not, these applications will not be able to exploit high-end computing systems likely to employ hundreds of millions of such cores by the end of this decade.

HPX is used for a broad range of scientific applications, helping scientists and developers write code that scales better and shows better performance if compared to more conventional programming models. This library enables application developers to write massively parallel, highly scalable codes using a modern multi-paradigm API. It facilitates distributed operations, enables fine-grained constraint based parallelism, and supports runtime adaptive resource management. In addition, HPX is portable as it supports heterogeneous runs on conventional and future architectures such as x86, Blue Gene, Xeon Phi, and ARM.

HPX is a novel combination of well-known ideas with new unique overarching concepts. It aims to resolve the problems related to scalability, resiliency, power efficiency, and runtime adaptive resource management that are of growing importance as high-performance computing (HPC) architectures evolve from peta-scale to exa-scale. It departs from today's prevalent programming models with the goal of mitigating their respective limitations, such as implicit and explicit global barriers, coarse grain parallelism, and lack of overlap between computation and communication. It exposes a coherent programming model, unifying all different types of parallel execution in HPC systems. While it is not based on any conventional programming model, it does integrate with those and provides a smooth migration path toward future computer architectures.

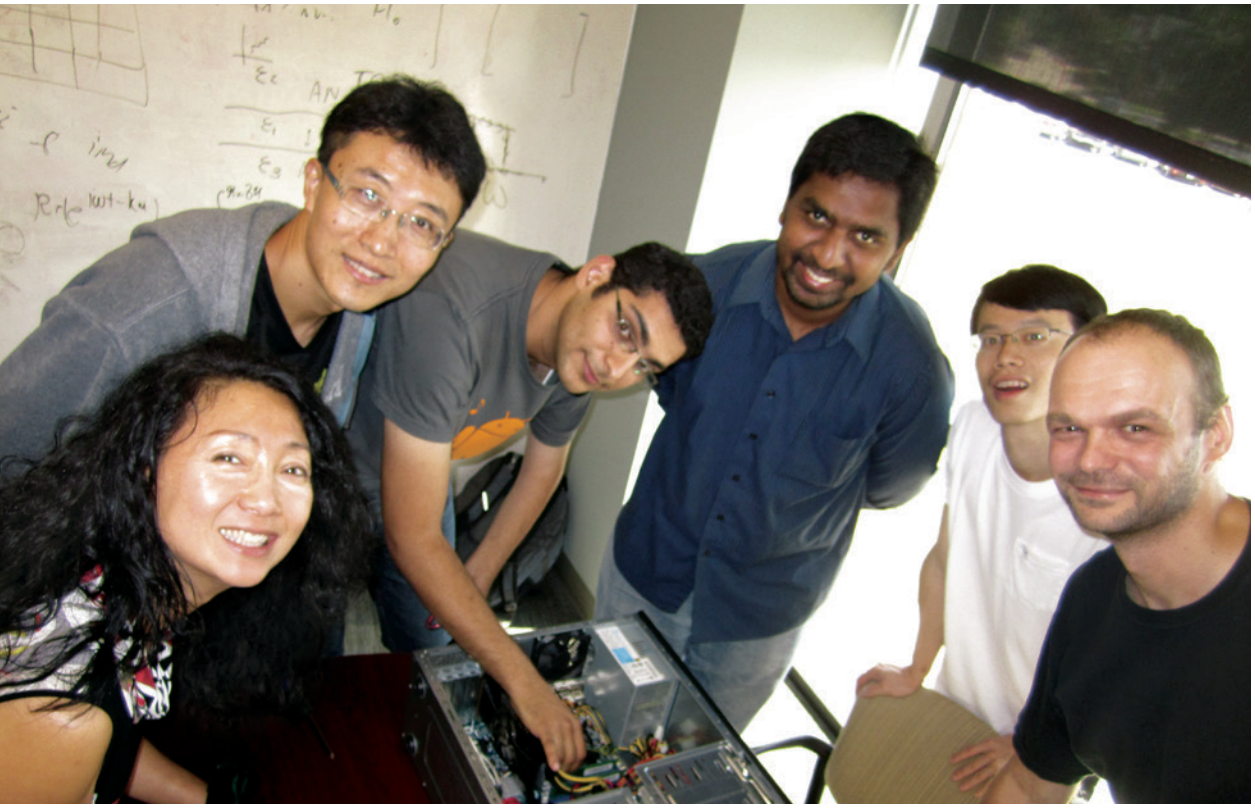
HPX represents an innovative mixture of global system-wide address space, fine grain parallelism, lightweight synchronization, and work queue-based, implicit message-driven computation, full semantic equivalence of local and remote execution, and explicit support for hardware accelerators.

In this release, HPX developers have improved the C++11/14 standards compliance, made parallel algorithms (proposed by working draft N4107) available to users, refactored the build system to support features such as static linking, and revamped our buildbot to discover and fix bugs sooner.

"The HPX v0.9.9 release provides the basis of a solution that will allow users to write simple, efficient, and portable code," said **Hartmut Kaiser**, lead of the STE||AR Group and senior research scientist at CCT. "These ideas will change the way applications are written and will one day be pervasive throughout the HPC community. HPX's portability and the compliance of the API to C++ lay the groundwork for its wide usability in different application domains."

See more at http://stellar.cct.lsu.edu.

TESC: Fostering Interdisciplinary Collaborations



Wei Feinstein, Jian Tao, Sameer Abu Asal, Rakib Hasan, Yun Ding, and Michal Brylinksi

Photo by Staci C. Kramer

The Technologies for Extreme Scale Computing (TESC) group is building on the interdisciplinary focus of the Center for Computation & Technology (CCT). TESC (pronounced tesk) includes more than 80 researchers, and its weekly meetings are attended by an average of 40 researchers.

Mark Jarrell, professor of physics and CCT Material World focus area lead, started the group in 2010. TESC, previously known as the GPU Team and Heterogeneous Computing Team, began in the Material World focus area and now includes members from all CCT focus areas.

The TESC group is funded by the Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA), a National Science Foundation-sponsored virtual organization of seven institutions of higher education focusing on computational materials science: Tulane, Xavier, the University of New Orleans, LSU, Southern, Louisiana Tech, and Grambling.

The interdisciplinary TESC team is devoted to the development of new computational formalisms, algorithms, and codes optimized to run on heterogeneous computers with graphic processing units (GPU) and recently Xeon Phi coprocessors. The team is focused on multiple projects, each devoted to the development of different codes, such as codes for simulations of spin glasses, drug discovery, quantum Monte Carlo Simulations, or classical simulations of molecular systems.

“Each project involves a collaboration of students from different domain sciences or engineering partnered with students from computer science or computing engineering,” said **Honggao Liu**, CCT deputy director. “We have found that this co-development model is ideal for the rapid development of highly optimized codes for GPU or Xeon Phi architectures.”

TESC now includes the Ste||ar Group developing HPX (see page 13), the Cactus Group (see page 20), and others at CCT interested in developing technologies for next generation supercomputing and big data analytics.

“One of the main goals of TESC is to graduate its researchers from serial and parallel computing to heterogeneous computing that will characterize the national leadership class capability computing in two to three years,” Liu said. “The TESC effort is very important for CCT and LSU.”

Researchers within the TESC group have collaborated on about 10 recent grant proposals, Jarrell said. "Funding agencies recognize we are providing new opportunities to do transformative research quickly," he said. "We combine disciplines for more opportunities in the cracks between the fields."

Michal Brylinski, assistant professor in the Department of Biological Sciences and CCT, is working within the TESC group on developing a new algorithm to speed up the discovery of new pharmaceuticals. There are hundreds of millions of drug candidates that could modulate the function of various macromolecules in a biological cell. Brylinski's project involves computer scientists, engineers, biologists, chemists, and physicists and uses the latest supercomputers to accelerate the process of drug development.

"It's like looking for a needle in a haystack, with a haystack that's just enormous," Brylinski said.

Although pharmaceutical companies may perform experimental high throughput screening to test millions of compounds, universities can't afford such large-scale experiments. So, Brylinski's team uses computer simulations to narrow down the number of compounds to be tested in a wet lab.

"Millions of simulations are no limitation for LSU because of our computing resources," he said. "Using molecular docking, or a simulation of what's happening in a cell, we can determine how well a drug and its protein target fit together, called the binding affinity. That allows us to weed out poor candidates and focus only on promising compounds."

"Our (TESC) students are trained to innovate, which is a perfect fit for companies focused on innovation."

—Mark Jarrell

This work requires highly optimized codes that run very fast, and within the TESC collaboration new codes targeting modern heterogeneous computing architectures have been developed that are accurate and ultra-fast.

The team is working with **Grover Waldrop**, professor in the Department of Biological Sciences and adjunct faculty member in CCT, to discover new broad-spectrum antibiotics. The possibilities for future applications are endless.

"A common theme of TESC is matching graduate students from domain sciences with those in computer science to work together on various projects across physics, biology, and chemistry," Brylinski said.

Education training and workforce development are important parts of the group, Liu said. "TESC researchers use next generation supercomputer architecture, giving students the chance to learn and gain experiences that are important to their future careers."

TESC students are able to secure internships at prestigious companies and national labs including Lawrence Livermore National Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, and Google.

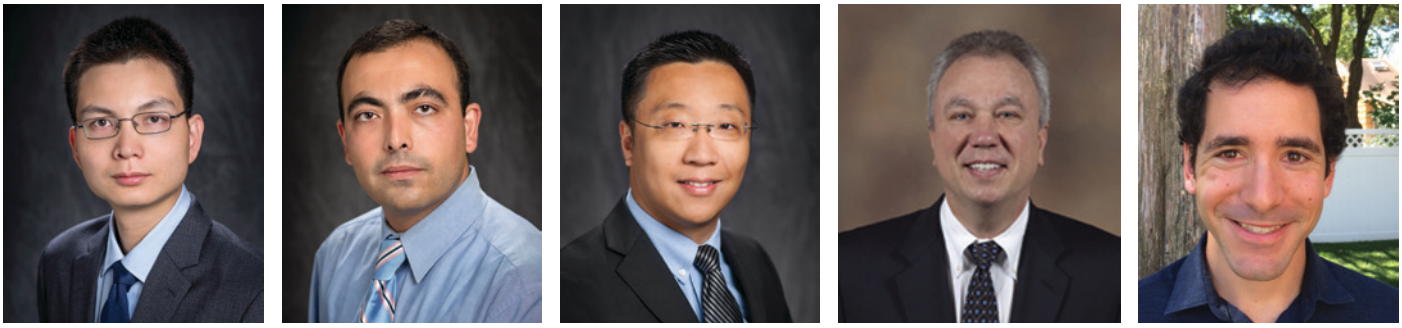
"Our students are trained to innovate, which is a perfect fit for companies focused on innovation," Jarrell said.

Wei Feinstein, CCT postdoctoral researcher, and **Jian Tao**, CCT research scientist, coordinate the TESC group.

The group meets every Thursday at noon in the Louisiana Digital Media Center and are provided free pizza and drinks at meetings that are open to the public and accessible remotely via video conferencing. Students provide progress updates on their work, and invited speakers give lectures about topics of broad appeal to anyone with an interest in scientific computing.

TESC has a wiki page at https://wiki.cct.lsu.edu/la-sigma/Main_Page and a project software package release page at http://institute.loni.org/lasigma/package/index.php for more information.

Strengthening Coastal Modeling Research with Five New Hires



Jun-Hong Liang, Celalettin Emre Özdemir, Zuo (George) Xue, Scott C. Hagen, and Giulio Mariotti

The Coastal Hazards Prediction and Mitigation (CHAPM) initiative at Louisiana State University welcomes five new faculty members. The initiative is a research cluster within the Department of Civil & Environmental Engineering (CEE), the Department of Oceanography & Coastal Sciences (DOCS), and the Center for Computation & Technology (CCT).

The new tenure track hires strengthen the collaboration among CCT, CEE, and DOCS on coastal hazards prediction and mitigation and complement the current strength of coastal modeling in the Coast to Cosmos (C2C) focus area at CCT.

Jun-Hong Liang, **Celalettin Emre Özdemir**, and **Zuo (George) Xue** joined the CHAPM group in fall 2014, and **Scott C. Hagen** and **Giulio Mariotti** will begin work in January 2015. Özdemir and Hagen have joint appointments with CEE and CCT, and Xue, Liang, and Mariotti have joint appointments with DOCS and CCT.

Liang's research interests are in oceanic boundary layer turbulence, air-sea gas transfer processes, mesoscale and submesoscale oceanic processes, and the role of these physical processes in controlling oceanic biogeochemical processes and marine ecosystem.

Özdemir's research interests are in environmental fluid dynamics, boundary layer turbulence in time-periodic flows, fluvial and coastal sediment transport, and high-performance computer modeling and simulations.

Using CCT's high-performance computing facility, Xue works on a coupled physical-biogeochemical model that attempts to qualify impacts of land use and climate changes on riverine inputs, mainly the Mississippi/Atchafalaya, and the structure and productivity of the marine ecosystem in the Gulf of Mexico.

Hagen's focus is on massively parallel, high-performance computational modeling of ocean, coastal, and inland shallow water flows and transport and ecological modeling, particularly with respect to coastal dynamics of sea level rise around Florida and in the northern Gulf of Mexico.

Mariotti's research goal is to understand the fundamental geomorphic mechanisms governing the morphological evolution of coastal environments and to predict their long-term trajectories under different scenarios. His research plan has two main directives: the study of coastal morphology using dynamical-systems modeling and the coupling between morphology and ecology.

The new hires join three existing coastal faculty members at CCT creating a more coherent and stronger research group: **Q. Jim Chen**, CEE/CCT professor, models coastal hydrodynamics and coastal hazards; **Robert R. Twilley**, DOCS professor and CCT adjunct faculty member, studies coastal ecology and flood risk assessment; and **Dubravko Justic**, DOCS professor and CCT adjunct faculty member, simulates hypoxia, with an emphasis on the Gulf of Mexico dead zone.

Chen is the CCT C2C focus area lead and served as the chair of the joint CCT/CEE/DOCS search committee. The CHAPM group is using high-performance computers to predict hurricane-induced coastal flooding, wetland erosion, hypoxia, and oil spills and developing strategies to mitigate the impacts of those hazards on coastal communities in Louisiana and beyond.

Researching the Sustainability of Mississippi River Delta Cities

The most populated cities in the world are located on deltaic coastal floodplains, their rich fertile soils and plentiful natural resources produce trillion dollar values. River deltas are disappearing at increasing rates because of human activity.

Photo by NASA

LSU researchers are working together in **Coastal SEES Collaborative Research: Changes in Actual and Perceived Coastal Flood Risks Due to River Management Strategies** to explore the relationships among human river management, sediment supply, wetland building capacity, coastal flood risk, and human perception of flood risk.

The project will focus on changes in coastal flood risks due to human manipulations of sediment delivery. The goal is to produce guidelines to use sediment to resolve challenges of relative sea level rise in deltaic coasts around the world.

The National Science Foundation named the project a 2014 Coastal Science, Engineering and Education for Sustainability (Coastal SEES) program award recipient in August. The project will receive $1,097,704. **Robert R. Twilley**, LSU Oceanography & Coastal Sciences professor and an adjunct faculty member of the Center for Computation & Technology (CCT), is the principal investigator. **Q. Jim Chen**, of the Department of Civil & Environmental Engineering and CCT, is a co-PI along with LSU's **Samuel Bentley**, **Nina Lam** and **Kevin Xu.**

"Deltas around the world are sites of tremendous environmental, economic, and cultural value, such as the Mississippi River Delta, and also some of the most vulnerable regions to impacts of sea level rise," Twilley said. "One of the most important adaptations is the management of sediment supply from rivers that can contribute to building land that compensates for effects of sinking. Our project will investigate the role of sediment management and reductions to coastal flooding from storm surge events as a way to design how people can adapt to such vulnerable coastal landscapes."

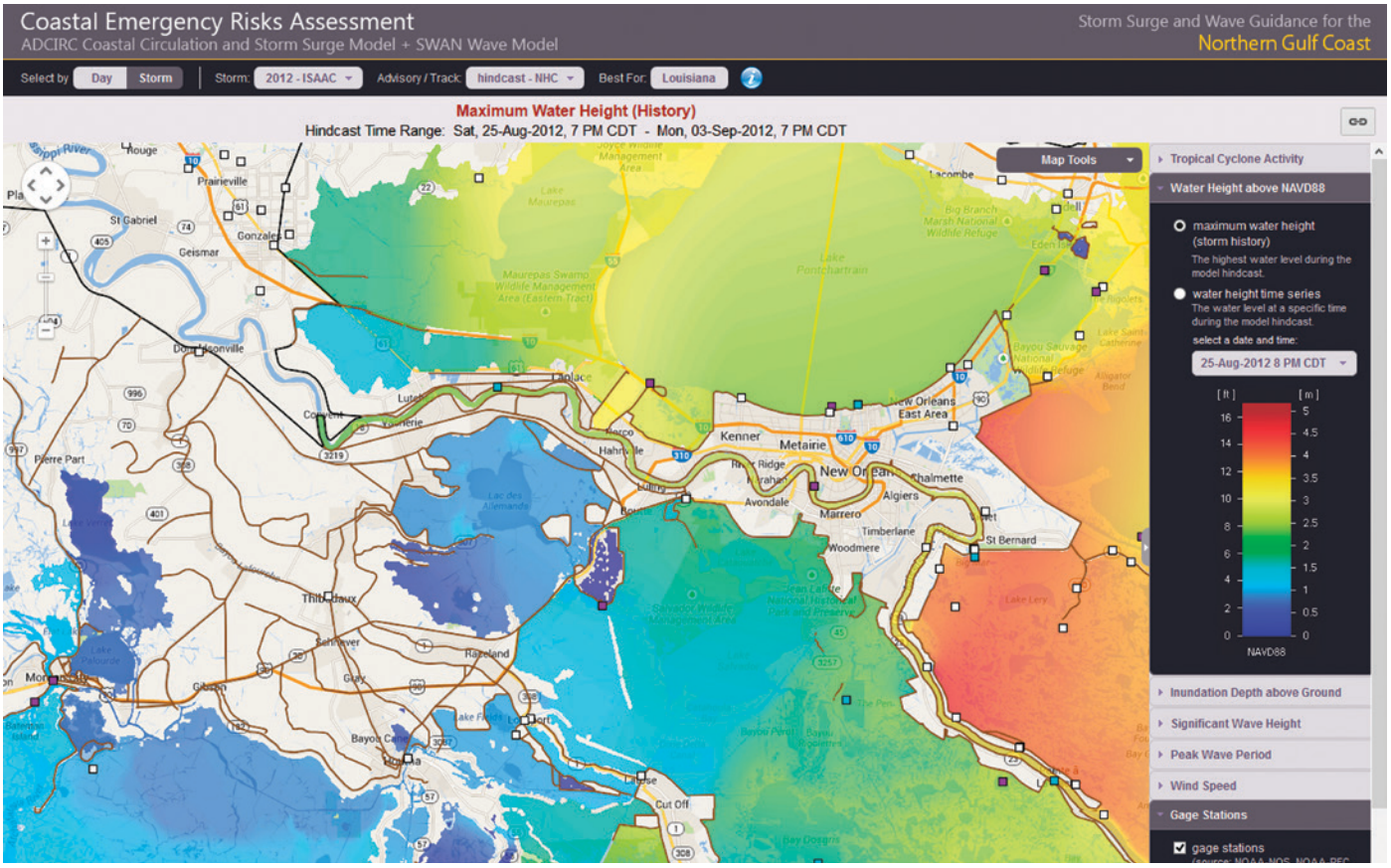
Three experimental coastal basins in the central Mississippi River Deltaic Plain with distinct histories of sediment delivery by rivers and wetland loss responses will be investigated. An interdisciplinary team of researchers will combine field studies and computer modeling approaches to characterize feedbacks between human river management strategies that reduce sediment delivery and corresponding landscape degradation and causal links between landscape degradation resulting from reduced sediment delivery, increased flood risks from hurricane storm surges, and human responses to perceived flood risks.

The team will explore historical and future outcomes of river management strategies, including how increased flooding risks have contributed to the reorganization of human settlements around changing landscapes. Computer simulations incorporating in what way reduced sediment supply causes wetland loss and by what means reduction in wetland areas can increase flood risks will be linked to studies of how humans perceive risks in low lying coastal areas. Testing these system interactions in a modeling framework will produce foundational knowledge that can inform management decisions and promote sustainable human settlements on deltaic landscapes.

Testing the connections among river management, wetland loss, and flood risks will improve prediction of future coastal system states and produce guidelines for how to sustainably manage sediment supply and maintain safer human settlement in coastal areas. High-performance computing systems at LSU will aid its researchers in achieving the research goal.

Other broader impact activities will include graduate and undergraduate education, application to public policy, and public and K-12 outreach. These are all unified through the general recognition in Louisiana (like many other deltaic coasts) that the science of deltaic restoration has strong and direct impacts on local welfare and economies.

STORM: Modernizing Storm Surge Prediction Software



Every year coastlines of the United States faces the threat of tropical storms and hurricanes. Accurately predicting their course and advance preparation for their landfall saves lives and property. Thanks to the innovative researchers at the Center for Computation & Technology (CCT) on **STORM**, a Scalable Toolkit for an Open community supporting near Realtime high resolution coastal Modeling, faster and more comprehensive tropical storm and hurricane forecasts will soon be available. Storm surge prediction software that has been utilized for decades is in the process of being upgraded with funds from a four-year grant awarded by the National Science Foundation this past August totaling $970,835.

The software, Advanced Circulation and Storm Surge model (ADCIRC), predicts areas that will flood during tropical storms and hurricanes and is a critical community resource used around the globe. ADCIRC addresses the effects and interactions of processes such as winds, tides, waves, and currents on water surfaces using the two-dimensional (vertically-integrated) and three-dimensional versions of the shallow water equations widely used in coastal modeling.

The project at CCT brings together a group of researchers from computer science, coastal science, and coastal engineering to broaden ADCIRC from a successful but somewhat static model based on a single, aging solution algorithm and parallelization strategy into a dynamic, multi-algorithmic modeling environment that takes advantage of recent transformational advances in parallel computing. The project combines coastal modeling and computer science research, sustainability, usability, and engagement.

STORM will sustain and improve ADCIRC by incorporating High Performance ParalleX (HPX) to parallelize code and run it on supercomputers. HPX is the first open source implementation of the ParalleX execution model and modern runtime system developed by the Systems Technology, Emergent Parallelism & Algorithm Research (STE||AR) Group housed at CCT (see page 13). Applying the ParalleX execution model will overcome limitations of ADCIRC's current implementation.

"While ADCIRC has worked capably in a number of applications in the

20 years since its development, we believe that its sustainability for the next 20 years requires the development and implementation of algorithmic improvements," said **Hartmut Kaiser**, CCT researcher, STE||AR Group lead, and principal investigator for STORM. "Ultimately ADCIRC will become more robust, faster, and much more scalable. Funding from the NSF is a major breakthrough for our work."

The code modernization will impact another CCT project, the **Coastal Emergency Risk Assessments** (CERA) website, which is a graphic display of ADCIRC simulations run at CCT. CERA is developed by LSU Sea Grant Director and CCT adjunct faculty member **Robert R. Twilley** and CCT's **Carola Kaiser**. The NSF grant will also support CERA as an efficient means of communicating critical data to decision makers during hurricanes and other emergencies.

Collaborators on the project include the original authors of ADCIRC, **Joannes Westerink** of Notre Dame; **Rick Luettich** of the University of North Carolina; **Clint Dawson** of the University of Texas; and Twilley.

The ADCIRC Surge Guidance System (ASGS), a real-time, open source software automation system for coastal ocean modeling using ADCIRC, will be used to test the STORM project's improvements to ADCIRC. Lead developer **Jason Fleming** wrote the software package that generates storm surge guidance in real-time for approaching tropical storms and hurricanes. CCT uses ASGS to automatically update CERA with new data.

See ADCIRC and ASGS in action on the CERA website at http://cera.cct.lsu.edu.

CERA: Sophisticated Storm Forecasting Tool

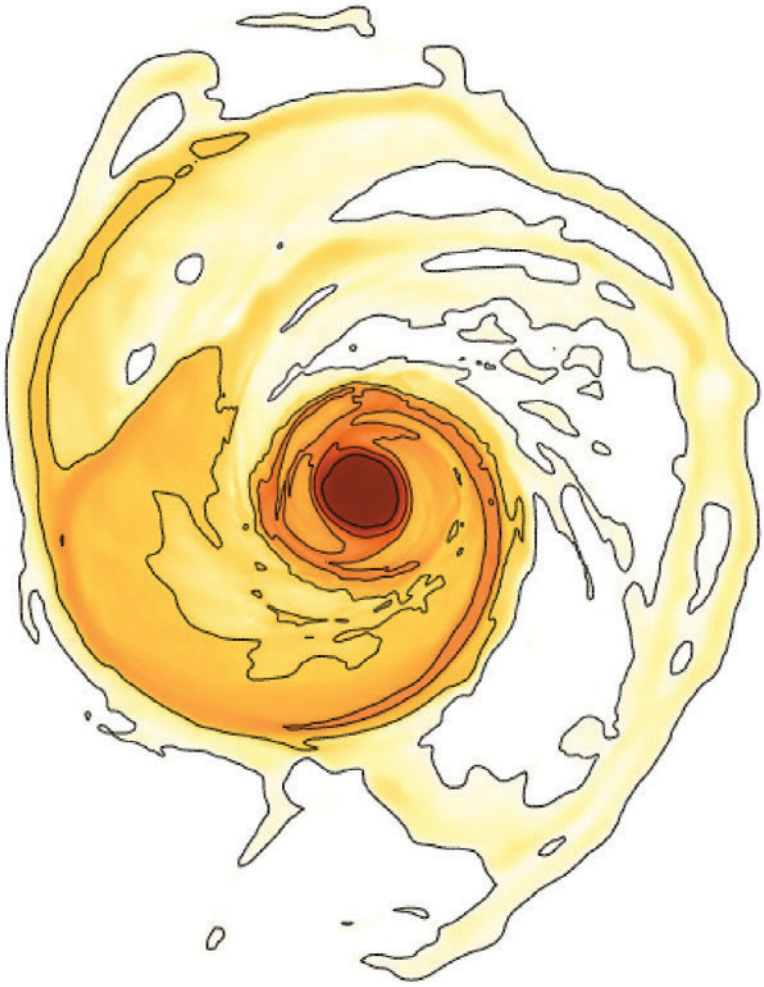
The LSU **Coastal Emergency Risks Assessment** (CERA) research group provides a sophisticated storm advisory system to local, state, and federal emergency managers and designated emergency responders for use during tropical storms and hurricanes. Available at http://cera. cct.lsu.edu, this real-time visualization website provides interactive predictions of wind speed, significant wave height, storm surge, water inundation above ground, and more that impacts the coastline of the United States during a tropical storm or hurricane's approach and landfall. The CERA web application allows emergency managers to quickly evaluate critical situations. Officials used it during hurricanes Irene (2011), Isaac (2012) and Sandy (2012).

CERA is supported by Louisiana Sea Grant, and the Center for Computation & Technology (CCT) provides the hardware support and fast network connections, which are key for the real-time system's seamless operation. Sea Grant Director and CCT adjunct faculty member **Robert R. Twilley** and **Carola Kaiser** of CCT developed the CERA storm visualization tool. **Zach Byerly**, a post-doc in the STE||AR Group at CCT, is the CERA operator who runs the underlying Advanced Circulation and Storm Surge (ADCIRC) model.

In September 2014, CERA launched daily forecasts for the National Weather Service created on an in-house, high-performance cluster at CCT. This year the group began using more servers housed at CCT in the Louisiana Digital Media Center. High-performance computing supercomputers housed on the LSU campus are utilized when a real storm comes.

This February a successful, two-day ADCIRC/CERA training was hosted by Sea Grant and the CERA group in collaboration with LSU Stephenson Disaster Management Institute. Twenty-seven workshop participants from the National Weather Service, Southeast Flood Protection Authority, as well as LSU, Mississippi State University, Notre Dame, and University of Erlangen personnel were taught how to create, run, and analyze a coastal regional model using ADCIRC. Participants were also taught how to successfully utilize the CERA website during active hurricane season. A second training is in the planning stages for spring 2015.

Astrophysical Simulations with the Einstein Toolkit



The figure shows the density contours of a slice through a rotating neutron star, after the onset of an instability.

By Steven R. Brandt

The Einstein Toolkit is a suite of codes used in relativistic astrophysics based on the Cactus Framework. This suite has been under development since 1997 and remains a powerful tool for studying black holes, neutron stars, and gravitational waves (ripples in space-time predicted by Einstein's theory of general relativity).

Some of the recent work with Cactus at the Center for Computation & Technology (CCT) centers on the collision of black holes of widely varying sizes. The Cactus Group at CCT includes **Frank Löffler**, **Peter Diener**, **Jian Tao**, and **Steven R. Brandt**.

Observations show that most galaxies contain super massive black holes in the center. It is also expected that smaller compact objects will be trapped in orbit around the central black hole, radiating gravitational waves. The small object will, therefore, lose energy and angular momentum, spiral in, and eventually fall into the big black hole. Such systems are expected to be one of the dominant sources of gravitational waves for future space-based gravitational wave detectors and are difficult to simulate numerically.

One of the main difficulties is that the emitted gravitational waves propagate on the curved background spacetime of the large black hole, partially back scatters and interacts with the small body at later times. Thus, the force acting on the small body depends not only on its instantaneous state of motion, but also on its entire previous trajectory.

The Cactus team is using the Einstein Toolkit to explore novel numerical techniques to simulate such astrophysical systems with the aim of being able to use gravitational wave observations to learn about the evolution of super massive black holes and their host galaxies.

The team has performed the first self-consistent evolution (i.e. the fields and particle trajectory evolved at the same time) for the simpler case of a scalar charge in orbit around a non-rotating black hole. The group is in the process of using these evolutions to compare with other approximate evolution methods in order to determine the accuracy of the approximations going into these methods.

The team has also started investigating the case of a gravitating small object, which brings in a whole other set of conceptual challenges to be overcome.

Another example of the toolkit's use is in the study of instabilities of neutron stars. These instabilities will be important to obtain information about the laws of physics and the behavior of matter in this regime. The environment close to this type

of star is so extreme that it cannot be reproduced in the laboratory, leaving these systems as one of the few places to directly learn about the laws of nature far from what we are used to on Earth.

Recent results obtained by collaboration between CCT and Parma University in Italy show the dependency of an important type of instability on the equation of state of these stars. In particular, more realistic equations of state show an earlier onset of the instability, with less differential rotation necessary than suggested by simpler equations that were used before. We also find that even in neutron stars that are rotating slower than necessary for the particular type of instability of the previous study, another type of instability can develop. Future studies need to confirm the theory that these are shear instabilities and to quantify their expected growth-times.

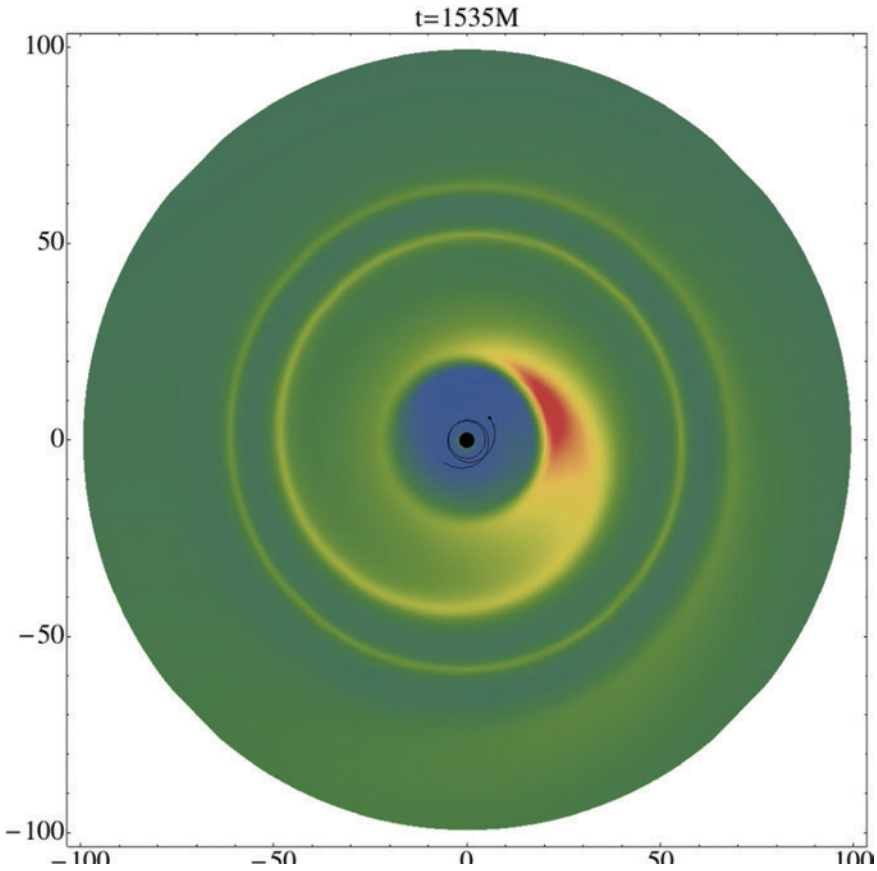
Once the team can reliably observe these instabilities, in part using gravitational waves, the researchers hope to be able to use these measurements and simulations to deduce matter properties in these extreme environments, effectively using these stars as laboratories.

For both black holes and neutron stars the theory of relativity is necessary, but the Einstein equations are too complicated to solve without the use of supercomputers, and they remain challenging even when using these powerful machines. Recently, the Cactus team has begun exploring ways to bring the power of the several decade old infrastructure to modern accelerators. The effort is called “Chemora” and seeks to exploit code generation to create a codebase that is better insulated against future disruptive hardware changes.

The Cactus Framework, however, isn’t limited to astrophysics. It is a general framework capable of evolving any set of hyperbolic or parabolic differential equations. Recently, it has been used to perform coastal simulations and the behavior of waves when striking levees, an issue close to the heart of the people of Louisiana.

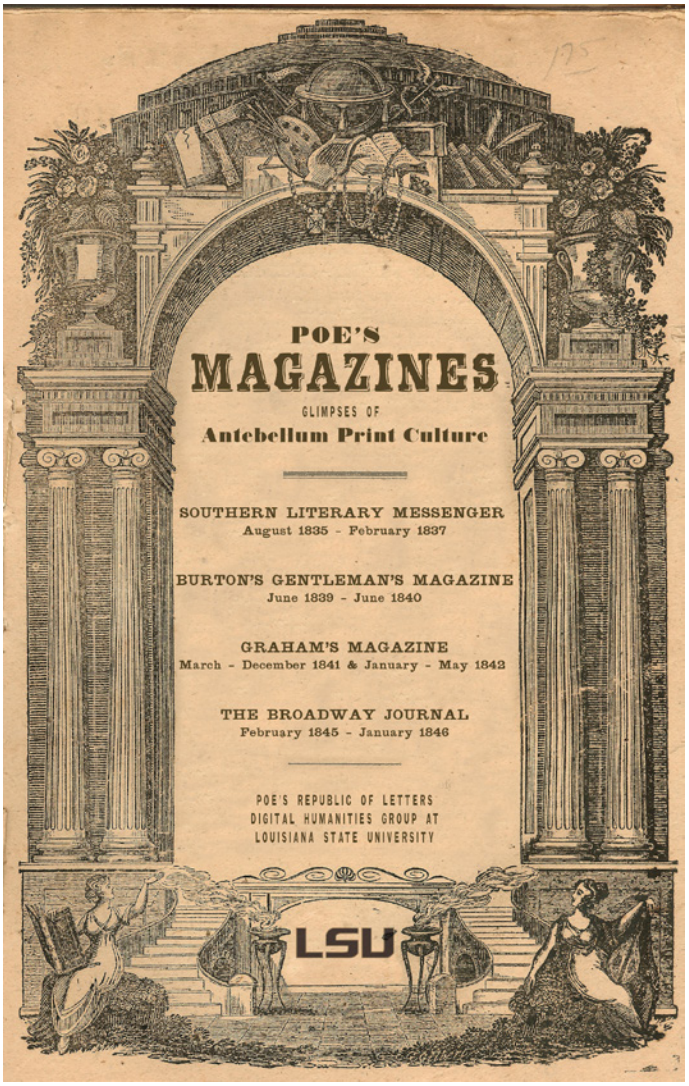
While Cactus has traditionally used regular grids and finite differences, a new framework is under development to integrate PHG (Parallel Hierarchical Grid). PHG is a finite element method (FEM) library developed by researchers from the Institute of Computational Mathematics Chinese Academy of Sciences. CaPHG takes advantage of the programmability of the Cactus computational framework and the performance and scalability of the PHG library to provide an integrated problem solving environment to solve large scale scientific problems with FEM and DG methods on high-end computing facilities.

Learn more at http://einsteintoolkit.org.



Equatorial snapshot of the scalar field produced by a scalar charge in orbit around a black hole. The central black dot shows the black hole. The smaller black dot shows the current location of the scalar charge and the line trailing it shows a part of the previous trajectory. Notice the spiral pattern in the wave traveling outwards.

CCT Digital Humanities Work to Digitize Poe's Magazines



"We hope to be able to apply these tools and techniques to today's digital culture and potentially apply them to science and mathematics, which are core to what we do here at CCT."

—Chris Branton

Researchers plan to put the computing power of the Center for Computation & Technology (CCT) to work in the humanities by digitizing a portion of Edgar Allan Poe's work.

Best known for his mystery tales and short stories, Poe (1809-1849) was also a magazine editor. Collaborators at Louisiana State University, including CCT, are constructing a searchable digital collection that includes every issue of four antebellum magazines edited by Poe.

The project, ***Poe's Magazines: Exhibiting Antebellum Print Culture***, will digitize 95 issues of the *Southern Literary Messenger* (1835- 37), *Burton's Gentleman's Magazine* (1839-40), *Graham's Magazine* (1841-42), and the *Broadway Journal* (1845-46), creating a 3,200 page treasure trove of data that reflects America's antebellum culture. The public will gain access to a reference resource containing the entire contents of those periodicals associated with Poe's career as a magazine editor.

"Our big idea is to create a digital archive devoted to antebellum print culture, built around Poe as an exemplary figure," said **J. Gerald Kennedy**, Boyd Professor of English at LSU. "His work helps us understand the network of relations in literary America at the time."

This inherently interdisciplinary work relies on researchers in the humanities, library and information sciences, and design. CCT provides underlying technology and information systems support.

So far, four sample issues have been scanned and processed, and a prototype site hosted at CCT launched October 1 at http://literati.cct.lsu.edu/poesmagazineworld.

The resulting resource will provide more than just a way to read the magazines digitally. Researchers will provide value-added content such as author biographies and authoritative previews of each issue, identifying significant contents and noting provocative cultural threads.

These periodicals open a window to antebellum America and provide a revealing exhibition of its preoccupations and curiosities.

"Magazines filled an important cultural role through the first half of the 19th century, similar to the role of television shows and the Internet today. Periodicals are our primary source for understanding the trends, tastes, and conflicts of the period – in art, religion, politics, and philosophy," said **Chris Branton**, IT consultant at CCT and adjunct professor in LSU's Department of Computer Science & Engineering. "This project will allow users a unique view of the culture of the mid-1800s in its original context, complete with advertisements and layout styles."

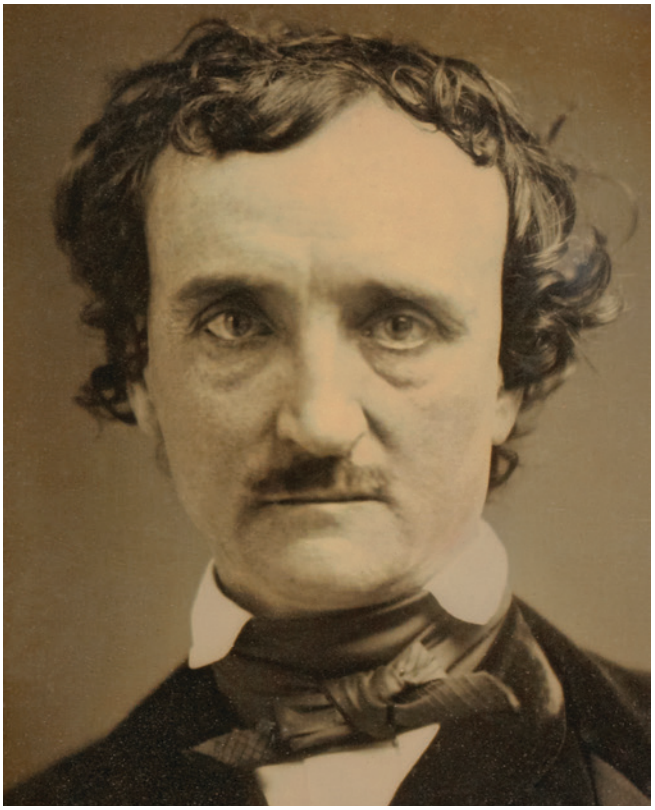
As a magazine editor, Poe had to fill the issues, and researchers suspect that oftentimes he would write articles anonymously, without credit, or under a pseudonym.

"Within the last year we have developed several tools to gather and analyze the structure of the text generated by the project," Branton said. "Analysis of the magazines' content should help us identify Poe's fingerprints of authorship."

Poe's Magazines will provide access to work that's nearly 200 years old. While the hard copies of the magazines are preserved and available in physical locations such as the LSU Libraries Special Collections at the Hill Memorial Library, the digital copies will allow even more readers access to them from anywhere in the world.

"The technology we're developing will allow new ways to explore and interact with the content," Branton said. "We can potentially discover connections within the content using computation that aren't easily perceivable through reading."

The project will have applications beyond Poe's work. "We hope to be able to apply these tools and techniques to today's digital culture and potentially apply them to science and mathematics, which are core to what we

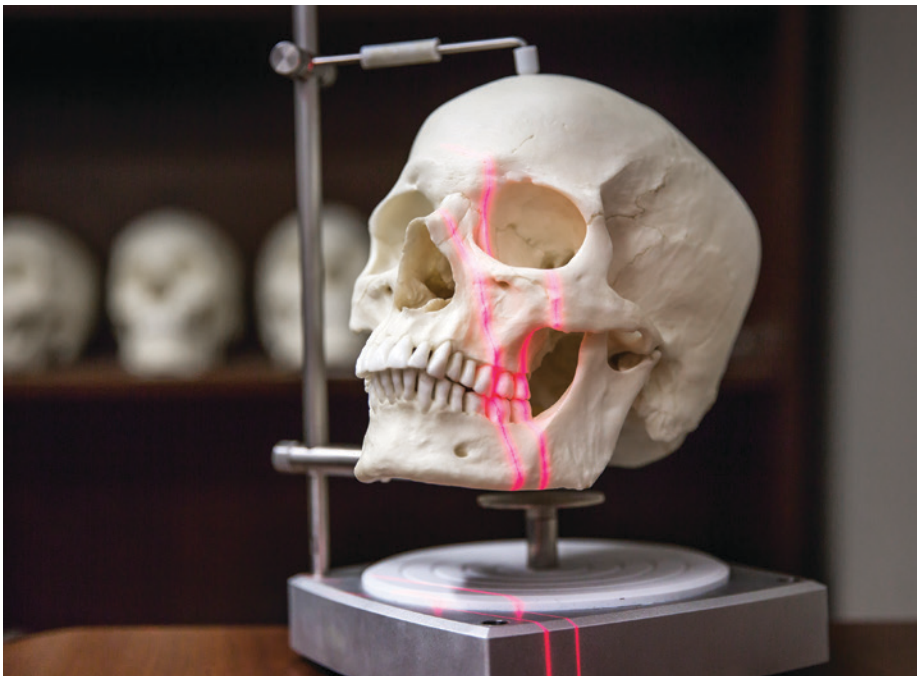


do here at CCT," Branton said. "For example we could examine datasets for specific types of data collection bias or research papers for relative contributions of authors."

The project will ultimately be folded into a larger digital archive being developed at LSU, *Poe's Republic of Letters*, and linked with an emerging grid of Americanist archives, a connectivity facilitated by the project's adoption of common formats and protocols.

"Scholarship will be done mostly or entirely online through explorations of digital archives like the one we're trying to create," Kennedy said. "Eventually seamlessly connected archives will allow researchers access to explore ideas, see connections, and have a richer awareness of the ways literary texts enable understanding of cultural context."

Puzzles Pieced Together with Geometric Data Mapping



A model skull with pink laser lighting from the 3D scanner.

Law enforcement officials use forensic face reconstruction to assist in the identification of skeletal remains. This process is not as easy as it is made to look on popular television programs that showcase forensic techniques; current procedures are relatively slow, expensive, and sometimes reliant on the interpretation of the forensic specialists' expertise. This work can be especially daunting if a portion of the skull is missing.

Work being done by **Xin "Shane" Li**, Oskar R. Menton Professor of Electrical Engineering and C. W. Armstrong Jr. Professor of Engineering in the School of Electrical Engineering & Computer Science and the Center for Computation & Technology (CCT), includes processes in a digital environment that uses cutting-edge 3D geometric modeling techniques that can recompose a fragmented skull and repair their damaged regions.

Moreover, additional processes enable skull assessment and facial reconstruction. This effort, in collaboration with **Mary Manhein** from the LSU Forensic Anthropology & Computer Enhancement Services (FACES) Lab, and **Warren Waggenspack** from the LSU Department of Mechanical Engineering, received funding from the Louisiana Board of Regents and the National Science Foundation in 2013.

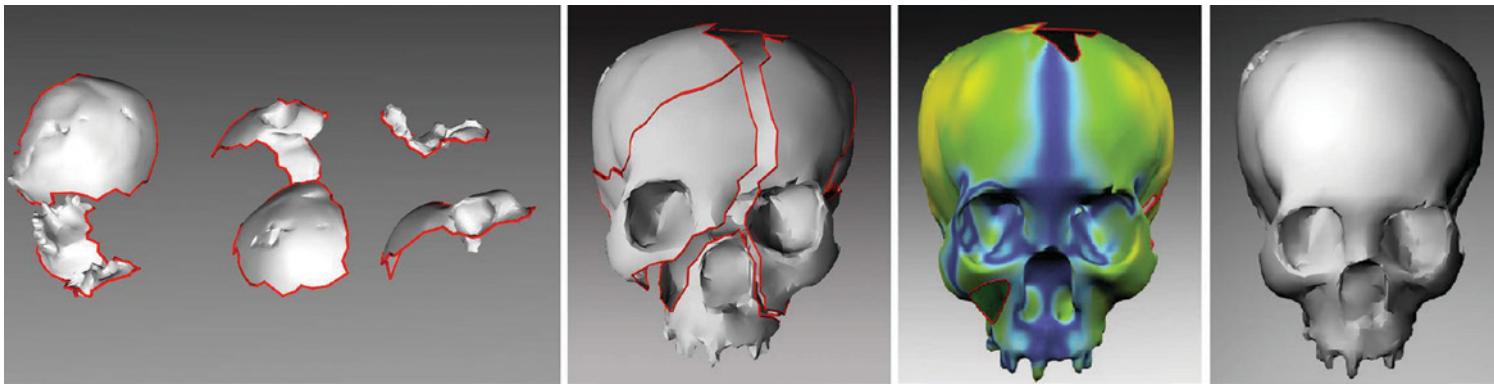
"We're able to do geometric data restoration from fragmented pieces of skulls, artifacts, and also broken documents in 2D," Li said. Recomposing a fractured skull is basically a puzzle problem, and Li said there are two approaches to such problems.

"One approach is to solve the puzzle following a template, if you have a few examples of complete objects that resemble the original shape to restore," he said. Li and his team are building a database of different skull shapes to serve as benchmarks. "The other approach is to align adjacent pieces using their matched geometric or texture patterns. We are developing pattern matching software programs that integrate both approaches to do efficient and automatic damaged data restoration."

Li and his Geometric and Visual Computing group conduct research on geometric data mapping and matching, which in addition to forensics, has many applications in medical research, archaeological tasks, and computer-aided design and manufacturing.

Li studies effective structural mesh generation, which constructs high-quality quadrilateral meshes for 2D regions or surfaces and hexahedral (cube-like) meshes for 3D solid geometries. Effectively generating such regular mesh can significantly improve the efficiency and stability of finite element computation in many computer-aided engineering problems and can produce critical parameterizations for the recently emerging Iso-Geometric Analysis (IGA) research (IGA aims to integrate finite element analysis into conventional computer-aided design tools).

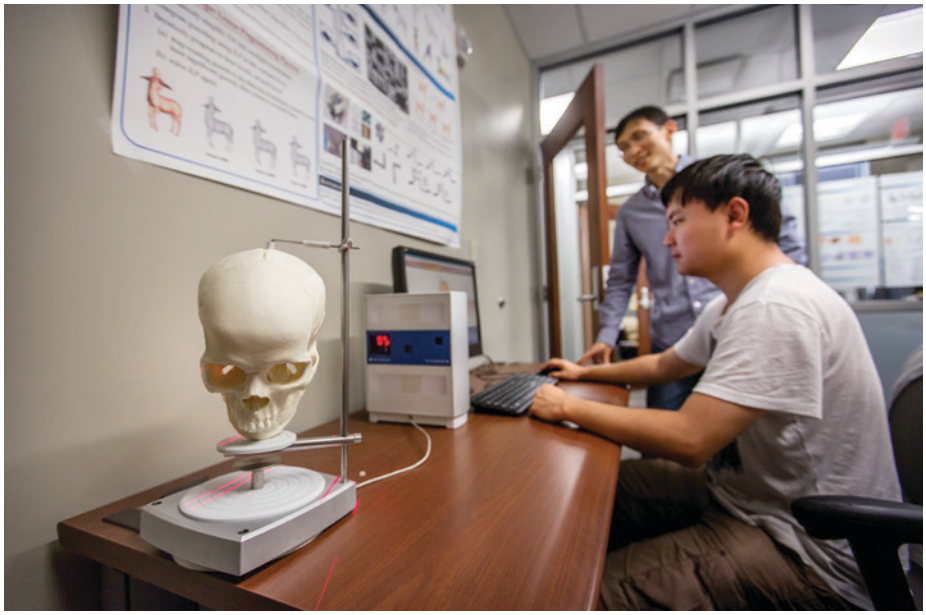
In collaboration with several medical centers, including the University of Texas Southwestern, Pennington Biomedical Research Center, and Mary Bird Perkins Cancer Center, Li's team has worked since 2010 on a lung tumor tracking problem,



which aims to develop a computer-aided system for next-generation radiotherapy treatment management. A lung tumor stays in motion during radiation treatment because the patient keeps breathing.

Li's work uses previous patient scans to create a parametric deforming model-to-model and predict the tumor's movement, target the radiation to just the tumor, and minimize damage to surrounding lung tissue. He is currently working to utilize high-performance computing to improve the speed before this tracking can be done in real-time. The Louisiana Board of Regents and IBM have funded this project.

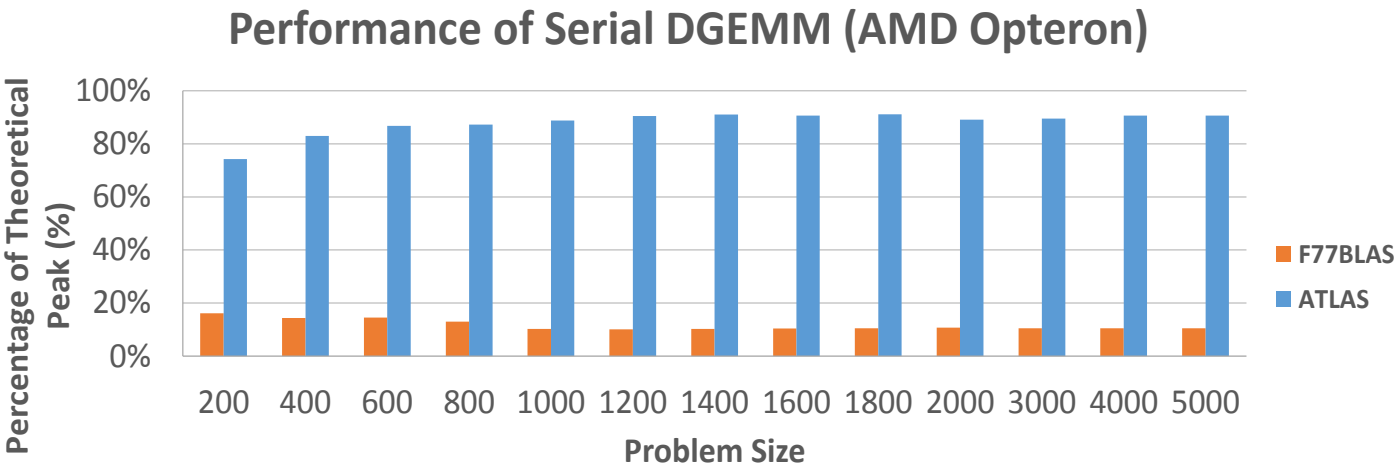
Working with **Dr. Steven Heymsfield**, Li's group has also developed a body scanning device at Pennington for diabetes analysis. Using several Microsoft Kinects (motion sensing input devices for game consoles) placed at multiple angles, this low-cost scanner only takes 3-4 seconds to scan and reconstruct a complete human body geometry within 1 cm accuracy. So far, more than 70 people have been scanned. Commercial laser body scanners can be more accurate but are slower and are also much more expensive – more than $120,000.



Top: Images showing Li's fragmented skull restoration algorithm, where several fragmented skull pieces are reassembled and repaired automatically. From left to right: (1) fragmented skull pieces; (2) fragment reassembly; (3) symmetry pattern analysis for skull completion; and (4) restored skull model.

Bottom: Xin "Shane" Li and his PhD student Kang Zhang complete a 3D scanning of a skull model to get its accurate 3D geometric model, the first step in the process of moving skull restoration and facial reconstruction into the digital environment

Improving Software Performance with ATLAS and iFKO



Comparison of the performance of untuned Double precision General rectangular Matrix Multiply (DGEMM) in orange and the performance achieved by ATLAS in blue on a 2.0 GHz AMD Opteron 6128.

For many simulations that are used in engineering and science, there is no such thing as "enough" computing power: added computing capability is used to increase the detail and accuracy of the simulation. There is need to have this type of software run as efficiently as possible even as the peak performance of the hardware continually improves over time.

Unfortunately, producing software that runs near the peak of the machine's capabilities is a much harder task than writing functionally correct programs. In general, it requires detailed understanding of all levels of the hardware and software stack to achieve extreme levels of performance. Compounding the situation, a program that is tuned to improve performance on one platform will often perform worse than one that has not been tuned at all when ran on another platform.

The software community has traditionally pursued two methods to optimize software performance: (1) it produces optimizing compilers that attempt to improve performance for all codes on all machines and (2) it provides performance-centric libraries that are hand-tuned for particular operations on particular machines.

For operations such as dense linear algebra, which underlie a host of scientific, engineering, and industrial applications, the hand-tuned code can often run orders of magnitude faster than using straightforward implementations compiled by general purpose compilers.

An associate professor in the LSU Department of Computer Science and the Center for Computation & Technology (CCT), **R. Clint Whaley** and his research group work on developing software frameworks that can achieve hand-tuned levels of performance automatically. This allows researchers and industry in many fields (computational sciences such as chemistry, physics, astronomy, engineering disciplines, medical imaging, movie special effects, etc.) to get access to the extremely efficient software their work demands.

There is typically almost an infinite number of ways to express a given computation. One way will be efficient on machine A, while a completely different implementation of the same computation will run much faster on machine B. When a hand-tuner tunes a given computation to a particular machine, he or she may write

"There's no such thing as enough performance. ATLAS tries to meet the need for maximum efficiency out of hardware in an automated way. We can see up to 100-fold speed ups with this kind of tuning."

—R. Clint Whaley

hundreds of implementations of the same computation, time them, and then keep the best.

In Whaley's research, this process is automated by creating software frameworks that can automatically transform input kernels in ways known to affect performance.

The frameworks further include search programs that can investigate all known transformations and complicated timers that replicate how computations are used in the real world. When installed on a new machine with unknown computational properties, the automated search process can empirically determine the effect of a code transformation on performance and retain only those variations that result in performance improvements on this particular kernel on this particular hardware. A kernel is any small routine that, when optimized, can speed up the overall performance of a much larger application.

Since the process is done automatically, hand-tuned levels of performance are seen in hours rather than weeks or months (or never, if you are using a kernel or computing platform that is not widely enough used to attract hand-tuning experts).

Whaley is pursuing the goal of providing high-performance software automatically with two research projects.

The first is Automatically Tuned Linear Algebra Software (ATLAS) that aims to automatically tune the widely used Basic Linear Algebra Subprograms and Linear Algebra PACKage libraries to arbitrary cache-based computer architectures.

ATLAS can produce highly tuned linear algebra routines for essentially any modern computer architecture, using a search and dedicated code generators to discover the best performing implementation for a new computer architecture.

In Whaley's latest ATLAS research, his team is investigating how to make ATLAS automatically handle extreme-scale shared memory parallelism.

When ATLAS was originally developed, typical shared-memory parallel machines had two to four CPUs, while very large machines might have eight. Due to trends in computer architecture, the number of CPUs has been recently going up strongly, with the newest Xeon PHIs essentially needing hundreds of parallel threads. This requires a new approach to parallelism, and Ph.D. student **Rakib Hasan** has been working with Whaley to drastically improve ATLAS's extreme-scale performance.

ATLAS is in use by scientists, engineers and industry world-wide, including researchers at LSU/CCT, and is freely available at http://math-atlas.sourceforge.net.

The main shortcoming of ATLAS is that it is dedicated to dense linear algebra. Linear algebra kernels underlie many high performance applications, but not all. Therefore, in iterative Floating-point Kernel Optimizer (iFKO) Whaley attempts to perform this level of tuning for any computational kernel.

iFKO is iterative, meaning it tries multiple things, and empirical, meaning it makes choices based on actual timings on the hardware being tuned for, compiler created for extreme tuning of computational kernels. The iFKO compiler presently targets x86 architectures. **Majedul Haque Sujon** is a Ph.D. student whose research is centered on iFKO.

New DMAE Master's Program Starts 2015

The DMAE program occasionally presents free film screenings and Cinema for the Ears Concerts in the Louisiana Digital Media Center theater.

Photo by University Relations

The new **Digital Media Arts & Engineering** (DMAE) master's degree program at LSU expects to welcome students in 2015. This is an intensive two-year degree program that will combine a practical and classroom experience to educate students who will be well-prepared to meet growing digital media industry needs. The program is part of the Center for Computation & Technology (CCT).

This program will offer innovative top graduate-level interactive, media and entertainment technology courses. Students will work on complex team-based projects solving problems using professional tools and pipelines. This professional program is designed to teach leadership, creativity, technical prowess, and design excellence in digital media. Students will learn cutting-edge technology and possess the practical experience to apply it.

"This is a professional, terminal degree that will prepare our students for careers in digital media," said DMAE director **Marc Aubanel**. "Through partnerships with professional entities, students will gain real-world experiences and learn more than just theory. Our program is studio-based with more time working on team-based projects and less classroom time." Students will work with a diverse group of digital artists, programmers, musicians, and researchers to develop their ideas into the future of media. DMAE courses will explore cutting-edge developments in video games, interactive design, visual effects, and animation.

This degree program is important to Louisiana and its economic development. The DMAE program will be the first digital media master's degree offered in the state, which has a $14 million digital media industry. Until now, Louisiana did not have a graduate degree program to train people for this vital sector. The program expects to admit 20 students annually.

The development of the DMAE program ensures that state and national digital media industry will be provided a source of employees with the skill sets conducive to digital media and software development. By addressing immediate industry needs where the knowledge demands on the workforce are increasingly becoming more technical in nature, the program combines artistic and scientific talent.

Digital media has been in the domain of engineering and the digital arts but has expanded into many other disciplines. With a rapid acceleration in gamification, low-cost portable

devices and app development, the possible fields affected by digital media is growing. It has relevance in mass communication, business development, communication studies, and architecture to name a few.

As of October 2014, the participating colleges, the Courses and Curriculua Committee and the LSU Graduate School approved the program. It is in the final stages awaiting approval by the LSU Board of Supervisors and the Louisiana Board of Regents.

Applications are being accepted now. Visit http://dmae.lsu.edu to learn more.

LSU's Connected Classrooms Set Model for Distance Learning and Event Recording

Louisiana State University's Center for Computation & Technology (CCT) has taken the lead for advancing communication technologies at the Louisiana Digital Media Center (LDMC). CCT is developing new techniques for visualization and achieving callorbration and teaching of the sciences and arts to support cutting-edge interdisciplinary research and development.

Part of that mission is carried out by having students, research staff, and faculty work on large-scale interdisciplinary projects in collaboration with national and international research groups. Utilizing videoconferencing for distance learning and collaboration is a core strategy of CCT.

To enable CCT to deliver lifelike full HD images, Sony BRC-H700 PTZ HD robotic cameras were installed in the LDMC's state-of-the-art 200-seat theater and two of its classrooms. These systems enable researchers and students to participate remotely, with a high quality interactive experience that serves as a model for academia and industry.

"CCT brings unique research, tools and infrastructure based on information technology to foster multi-disciplinary research and education," said **J. "Ram" Ramanujam**, CCT's director. "We appreciate Sony's leadership in HD camera technology and how it is helping us improve communications across both professional disciplines and geographic boundaries."

Plans for the LDMC were drawn up in 2010, but the communication infrastructure for it had come together a decade earlier. The Louisiana Optical Network Initiative (LONI), a statewide project to provide a high speed Internet backbone for the state's industry and academic infrastructure, created ample bandwidth connecting LSU in-state, nationally, and globally. The new facility offers the opportunity to fully realize the potential of the high speed interconnects.

The first year of operation with the BRC-H700's has been a success.

"The classrooms and theater are in constant use, and the quality and consistency of the imaging has lived up to expectations," said **Adam Yates**, IT manager for CCT. "These classrooms are especially crucial for our work with other schools that are part of the LONI member network. They are also being adopted as a model for others locally here at LSU as well as nationally and internationally."

AVATAR Digital Media Minor

Photo by Robert Kooima

Developed and led by CCT, LSU's Arts, Visualization, Advanced Technology and Research (AVATAR) digital media minor has 94 undergraduate students from colleges across the campus participating in a multi-disciplinary program that helps prepare students for jobs of the future. The minor includes classes that challenge computational thought, artistic expression, and interactivity. The College of Engineering, College of Art & Design, College of Music & Dramatic Arts, E.J. Ourso College of Business, and the Manship School of Mass Communication offer classes in this minor. More than 35 students have completed the minor and graduated since AVATAR's inception in 2010. Enrollment in the minor grew quickly with the number of students entering the program quadrupling in its second year.

LSU Hosts Google Summer of Code Research

More than 1,200 student developers from all over the world received financial support from Google this past summer to produce code for open source projects as part of the company's prestigious 2014 Summer of Code program. Since it began in 2005, Google Summer of Code has trained 7,500 student participants from 97 countries and more than 7,000 mentors from 100 countries, resulting in at least 50 million lines of code.

Two student participants worked with researchers in the Center of Computation and Technology's (CCT) **Systems Technology, Emergent Parallelism & Algorithm Research** (STE||AR) Group. This group was selected as a host organization - one of only 190 approved worldwide.

Student applicants accepted into the program were each paired with a mentor. Student participants gained valuable experience with real-world software development scenarios and the opportunity for potential employment opportunities in areas related to their academic pursuits. In turn, the participating projects were able to more easily identify and bring in new developers. Best of all, more source code is created and released for the use and benefit of all.

Student participant **Anuj Sharmer** worked with **Hartmut Kaiser**, senior research scientist at CCT and STE||AR Group leader, to create a distributed vector for HPX (High Performance ParalleX).

Student participant **Christopher Bross** worked with **Andreas Schäfer**, STE||AR Group member and researcher at the Friedrich-Alexander University of Erlangen (Germany), to implement a sparse matrix container and an unstructured grid for LibGeoDecomp, an auto-parallelizing library to speed up stencil code-based computer simulations.

"Google's decision to support our group recognizes the importance of our research in the area of distributed parallel computing," Kaiser said. "This technology has the potential to transform the way we program and run applications today and to massively increase the possible parallelism and thus the efficiency of our codes."

Summer of Code is designed to allow students to work remotely. Each student received a $5,500 stipend from Google for their work, and each mentor received $500 and funds for travel to attend the Google Summer of Code Mentor Summit at Google's headquarters.

"We were delighted to have the opportunity to work with bright, self-motivated students," said **Adrian Serio**, the scientific program coordinator for the STE||AR Group. "Google Summer of Code not only provides open source projects such as HPX a chance to accomplish some of our project goals, but also provides student participants the ability to partake in the cutting-edge computer science development happening here at LSU and elsewhere around the globe."

The STE||AR Group looks forward to continuing its work with the Google Summer of Code program to help foster the next generation of computer programmers.

New Computational Math Concentration for Undergraduates

Benjamin Birk, Rachael Keller, and Bruno Beltran

Photo by Susanne C. Brenner

The first three students will graduate with a new concentration in computational math from Louisiana State University in spring 2015. This new undergraduate concentration was created under the initiative of the faculty in the Core Computational Science focus area at the Center for Computation & Technology (CCT) who have joint appointments with the LSU Department of Mathematics.

To complete a degree with this concentration, students must complete four courses: numerical linear algebra, numerical differential equations, numerical analysis, and optimization. The students are also encouraged to have a summer research experience before graduating.

Benjamin Birk worked at Microsoft Research over the past two summers. He will be employed by Microsoft after he graduates with a double major in computer science and math.

Bruno Beltran, a math major, worked in a biology lab at Yale University over the past two summers and will be returning there for the spring semester as a research tech. He intends to apply to graduate school.

Rachael Keller worked at Pacific Northwest National Laboratory over the summer on national security projects. Also a math major, she plans to graduate with three minors, computer science, mechanical engineering, and Chinese. She plans to apply to graduate school.

Other students interested in the computational math concentration should contact **Susanne C. Brenner**, Core Computational Science focus area lead at CCT.

Summer Camps Encourage Students to Explore STEM

The halls of the Louisiana Digital Media Center at LSU were filled this summer with children excited about science, technology, engineering, and mathematics (STEM). The faculty and staff at the Center for Computation & Technology (CCT) realize the importance of attracting students into STEM disciplines. As part of our outreach efforts to K-12 students, CCT hosted seven different day camps for nearly 200 participants.

Campers at Alice in Computation Land

Alice in Computation Land

The fourth Alice in Computation Land camp was held June 9-13 for girls entering grades sixth through eighth who were interested in learning more about computational science and technology. Twenty-nine campers learned how to use computer applications in their daily lives and about careers available in the world of science and technology. The girls also learned about web page creation, animation, programming, computer modeling and simulation, and best practices for using the Internet. The Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA) co-sponsored the camp.

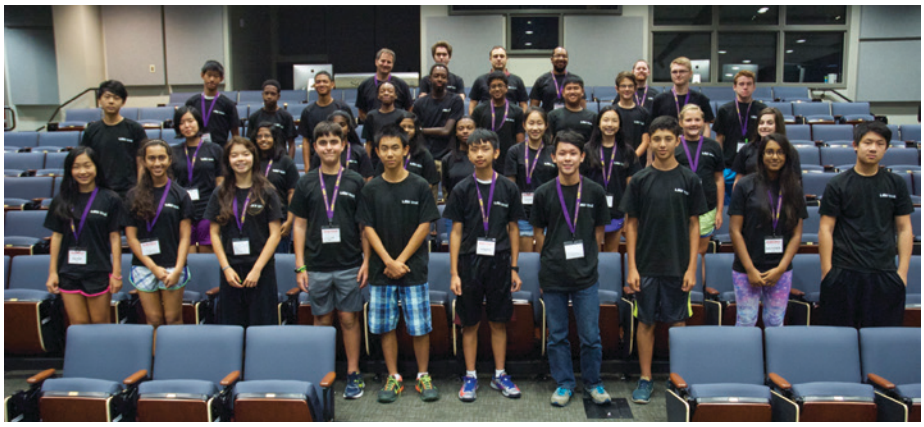
Danny Holmes makes sound adjustments in the Louisiana Digital Media Center theater during Girls Rock! Sound Engineering Camp.

Girls Rock! Sound Engineering Camp

Twenty-eight girls entering grades sixth through ninth attended the Girls Rock! Sound Engineering Camp hosted by CCT June 16-20. The camp incorporated sound engineering concepts with composition and live performance with technology. Campers made music with iPads, electronic instruments, and computers; recorded, edited, and sequenced sound; composed their own music; and designed cinema for the ears. The girls collaborated on a scientific visualization, each composing 45 seconds of music and sound effects for space imagery. The video and other images from the camp are available at http://emdmacademy.music.lsu.edu. CCT's **Jesse Allison**, assistant professor of experimental music and digital media, led the camp along with LSU student, **Danny Holmes,** and local St. Luke's Middle School teacher, **Alicia Lewis**.

PyFUN Programming Summer Camp

Boys and girls entering sixth through eighth grade participated in the PyFUN Programming Summer Camp, co-sponsored with LA-SiGMA July 21-25. During this programming journey 29 campers unlocked the power of Python, a general-purpose, high-level programming language. Using a fun, step-by-step approach that makes coding easy and exciting, students learned the basic concepts of programming including problem solving; computer parts and how they work together; syntax, strings, and console output; conditionals and flow control; functions, lists, dictionaries, and loops; introduction to classes; and file input and output.



Campers at the Gamecrash: Adventures in Game Design Camp

CCT's Derick Ostrenko provides a demonstration during a summer camp.

Gamecrash: Adventures in Game Design Camp

Marc Aubanel, director of LSU's Digital Media Arts & Engineering program, taught 31 high school students how to build videogames at the Gamecrash – Adventures in Game Design Camp held July 14-18. In its first year, the camp used video games (a subject matter students like) to encourage them to program and use geometry and physics – tools that they may not use otherwise. After working together to recreate two mini-games, the rest of the week was spent working in groups of three to five to create their own games from scratch. They created 10 unique games, which were played and critiqued by other high school students. Campers learned tricks and techniques used to make modern video games from scratch, professional tools to produce quick and easy gameplay prototypes, practiced scripting, animating, and digital art creation as well as level and game design, and unleashed creative potential to get ideas onto the screen.

Beowulf Boot Camp

July 7-11 CCT hosted the seventh annual Beowulf Boot Camp. The camp is named for Beowulf supercomputer clusters, which are made by connecting several regular computers. Thomas Sterling and Donald Becker at NASA invented the Beowulf supercomputer in 1994. This exciting camp offered 35 high school students, Baton Rouge Community College (BRCC) students, and teachers a unique opportunity to work with advanced technology. Camp participants learned how to build and use supercomputers as they worked hands-on with CCT faculty and staff including **Steven R. Brandt**, **Q. Jim Chen**, **Brygg Ullmer**, and **Peter Diener**. Campers built a computer cluster from scratch, installed the Linux operating system, connected the computers to make a mini-supercomputer, learned how to program the mini-supercomputer in parallel with Python, how parallel computing works in supercomputing, and ran performance benchmarks to rank their clusters against the fastest and largest supercomputers in the world. LA-SiGMA, DataDirect Networks, and NVIDIA co-sponsored this camp.

Middle School Science Fair Outreach

Andrew Knott, a middle school student at the Kenilworth Science and Technology Charter School in Baton Rouge, worked with CCT's **Shawn Walker**, assistant professor in the Department of Mathematics and CCT, on his project for the Louisiana Region VII Science and Engineering Fair in February 2014.

Knott's project, "Surface Tension," took third place in the Mathematical Science category. The Region VII area includes schools in East and West Baton Rouge, East and West Feliciana, Ascension, Iberville, and Pointe Coupee parishes.

Campers at the Baton Rouge Energy Venture Camp

Baton Rouge Energy Venture Camp

In partnership with Shell, LA-SiGMA, Gulf South Solar, Baton Rouge Community College, Dunham School, and LSU PERTT Lab, CCT hosted 31 high school students and one teacher for the Baton Rouge Energy Venture Camp held July 28-August 1. The camp, led by the Dunham School in Baton Rouge teachers **Jeannette Thompson** and **Richard Hansen**, was designed for students to learn about careers in energy while having fun. Students were able to perform many hands-on experiments to explore the entire process of energy development: from how oil and natural gas are formed to the ways various types of energy are used. They built a generator, motor, car, windmill, solar house, and robot and learned basic programming and simulations and about photosynthesis, distillation, catalysts, pressure, temperature, density, fracking, combustion, and how engines and superconductors works. Campers had unique hands-on experiences at the LSU Petroleum and Chemical Engineering labs, CCT, and the BRCC Process Technology (PTEC) lab.

Computer Math Summer Camp 2014

CCT welcomed 15 students entering eighth grade to the Computer Math Summer Camp held July 28-August 1. This new camp, co-sponsored with LA-SiGMA, highlights the strong connections between mathematics and programming. The camp leader was **Fernando Alegre**, a computer science instructor at Baton Rouge Community College. Activities reinforced math that students have already learned by presenting this knowledge in the context of computing. Campers learned about state-of-the-art functional programming, solved math problems using computers, practiced communicating mathematical ideas in precise language, learned how to use algebra and geometry software, and taught math to computers that "forgot" the subjects.

CCT Research Staff Voluntarily Teach LSU Courses

A number of staff members at the Center for Computation & Technology (CCT) voluntarily teach courses at LSU and oversee independent studies and dissertation research, mainly for the computer science department.

Class	Instuctors	Semester
CSC 1254 Computer Science II with C++	Hartmut Kaiser	Spring 2015
CSC 3102 Advanced Data Structures and Algorithms	Frank Löffler and Rahul Shah	Fall 2014
CSC 7700 Scientific Computing	Frank Löffler, Steven Brandt, Hartmut Kaiser, Peter Diener, and S. Jha	Fall 2014
CSC 2700 Scientific Computing	Frank Löffler and Kathryn Traxler	Spring 2014
CSC 4243 Interface Design and Technology	Chris Branton	Spring 2014
CSC 4700 Multiprocessor Programming	Steven Brandt	Spring 2014
CSC 1254 Computer Science II with C++	Hartmut Kaiser	Fall 2013
CSC 2700 Computational Science	Kathryn Traxler	Fall 2013
CSC 4700 Multiprocessor Programming	Steven Brandt	Fall 2013
CSC 7700 Scientific Computing	Steven Brandt	Fall 2013

Research	Instuctors	Semester
CSC 7999 Independent Study	Chris Branton	Fall 2014
CSC 9000 Dissertation Research	Hartmut Kaiser	Fall 2014
CSC 3991 CSC Honors Research	Chris Branton	Spring 2014
CSC 3999 Undergraduate Independent Study	Steven Brandt	Spring 2014
CSC 3999 Undergraduate Independent Study	Chris Branton	Spring 2014
CSC 4999 Independent Study	Steven Brandt	Spring 2014
CSC 7999 Graduate Independent Study	Chris Branton	Spring 2014
CSC 7999 Independent Study	Steven Brandt	Spring 2014
CSC 9000 Dissertation Research	Steven Brandt	Spring 2014
CSC 9000 Dissertation Research	Steven Brandt	Spring 2014
CSC 9000 Dissertation Research	Hartmut Kaiser	Spring 2014
CSC 4999 Independent Study	Steven Brandt	Fall 2013
CSC 9000 Dissertation Research	Steven Brandt	Fall 2013
CSC 9000 Dissertation Research	Hartmut Kaiser	Fall 2013

Supporting Research Experiences for Undergraduates, High Schoolers, and Teachers

CCT and LA-SiGMA REU and LA-SiGMA RET participants and mentors Steven Dorsher, David Koppelman, PI Juana Moreno, Morgan Burcham, Chris Branton, Katie Gamble, co-PI Jesse Allison, Lauren Lorio, Lia Klein, Shawn Liner, Natasha Navejar, Jackie Searcy, Kristen Barrett, Daniel Lauriola, Fortino Garcia, Brad Burkman, Josef Baylis, Jon San Miguel, Joel Montano, Jonathan Heath, Les Butler, Simón Lorenzo, Carsten Sprunger, Chris Hynes, NSF Division Director of Advanced Cyberinfrastructure Irene Qualters, and Debra Borskey.

Attracting students to careers in science, technology, engineering, and mathematics is a core goal for the Center for Computation & Technology's (CCT) outreach. An important way we work toward that goal is through our **Research Experience for Undergraduates** (REU) program.

Chosen from 150 applications, 10 students from across the country came to CCT at LSU this summer for a 10-week REU session. The program, funded by the National Science Foundation (NSF), is in its fifth year at CCT. Five additional REU students at CCT were funded by the **Louisiana Alliance for Simulation-Guided Materials Applications** (LA-SiGMA), which also supports REU students at other universities across Louisiana.

LA-SiGMA also provided funding this summer for four 11th graders in the **Research Experience for High School Students** (REHSS) and eight teachers in the **Research Experience for Teachers** (RET). These programs run for six weeks over the summer, overlapping the longer REU program.

"I really enjoyed participating in the REU because it was my first research experience and has been a big part of my motivation to continue my education by applying for graduate school."

—Shane Lindemann, LA-SiGMA REU student 2011

In the programs' first five years, 82 undergraduates, seven high school students, and 37 teachers have gained research experiences at CCT.

Each participant is paired with an LSU mentor to work collaboratively on a wide variety of computational science projects. This combination of individual training and immersion in a multidisciplinary research group provides rich research experiences in computational science. LSU mentors direct the research experience for students, while the RET participants come to campus with a research idea specific to their classroom needs.

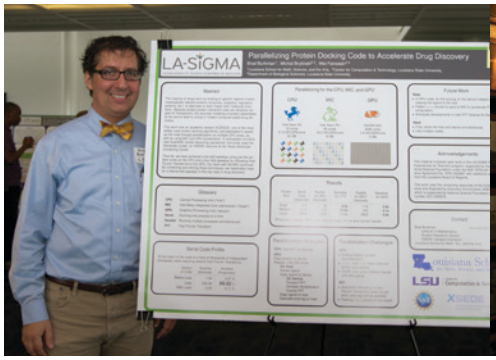
LSU has 12 other undergraduate research programs each summer, with about 150 students on campus in total. The CCT REU students are included in the joint activities, such as the welcome, orientation, the softball game, and several trip opportunities. A CCT-specific seminar series allows faculty mentors to share their research and careers.

These successful programs at CCT are made possible by the efforts of **Juana Moreno**, who is the principal investigator of the NSF CCT REU and co-principal investigator of the LA-SiGMA award. Both of these awards fund the research experiences. CCT's **Jesse Allison** became co-PI of the CCT REU award this summer, **Bety Rodriguez-Milla** and **Kathryn Traxler** serve as program coordinators.

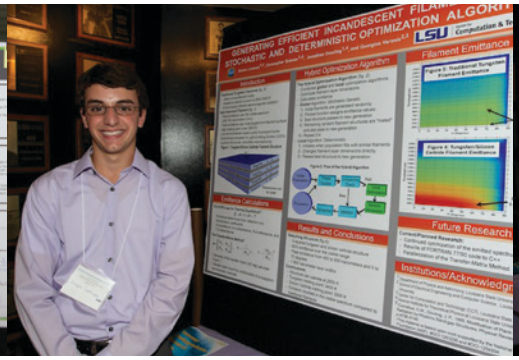
"CCT provides an ideal setting for the research experience of students and teachers, so they

Lia Klein (CCT REU), Natasha Navejar (LA-SiGMA REU), and Carsten Sprunger (CCT REU) during final presentations lunch.

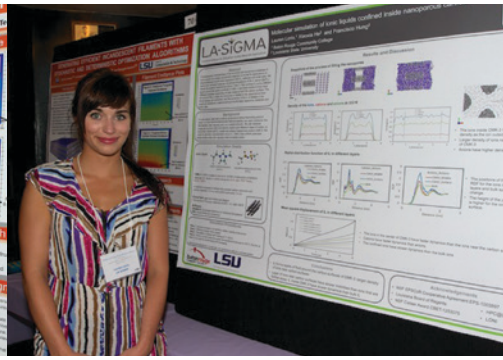
Photos by Bety Rodriguez-Milla



LA-SiGMA RET participant Brad Burkman



CCT REU participant Simón Lorenzo



LA-SiGMA REU participant Lauren Lorio

become familiar with interdisciplinary research," Moreno said. "With research groups exploring gravitational waves, complex emergent phenomena in material science, or computational music, the participants work on cutting-edge research in computational sciences."

The students learn how to use the most current cyberinfrastructure tools with individually designed training sessions targeted to their specific degree of preparation. **James Lupo**, CCT assistant director of computer enablement, teaches an optional programming class, and students are encouraged to engage in high-performance computing workshops to gain supercomputer knowledge. In addition, because most CCT research groups collaborate with international researchers, REU students and RET teachers learn how international collaborations work.

"I'm … doing software performance analysis in high performance computing; every job I've had has come out of the work in the REU."

—David Poliakoff, CCT REU student 2010 and 2011

"My research experience with CCT and REU was amazing."

—Sharae M. Williams, CCT REU student 2011

REU students end their summer with a final oral presentation and a poster presentation at the **Summer Undergraduate Research Forum** (SURF). REHSS participants' experience mimics the undergrads' without the final presentations.

CCT REU is supported by NSF grant OCI-1263236, and LA-SiGMA REU is supported by NSF award EPS-1003897. Application submission opens December 1 for the following summer, and the deadline to apply is March 1. See http://reu.cct.lsu.edu and http://reu.lasigma.loni.org.

LSU iOS App Boot Camp 2014

Thirteen participants came to campus August 4-15, 2014, to take part in the Center for Computation & Technology's (CCT) fourth annual iOS App Boot Camp, a 2-week training that gave campers the opportunity to learn and enhance their entrepreneurial spirits.

Working in groups, six LSU students, one LSU faculty member, one high school student, and five Electronic Arts employees learned application development processes and techniques for iOS, the operating system for Apple products.

The campers created four iOS apps: Tip-Assist, Hot Potato, Koasati Language Quizzes, and Interactive Lecture Notes. Participants also learned about mobile apps' business market, trends, and opportunities. Leading the course were CCT's **Jesse Allison**, **Robert Kooima**, and **Tim Wright**; each push the boundaries of mobile applications in computer science and digital media fields.

CCT's Mobile [App | Art | Action] Group, or MAG, meets throughout the year and builds on the work done at the boot camp. MAG is a forum to further thought and development with mobile platforms. Participants come together to share their progress, receive feedback and help, connect with others, and get inspired to try innovative things with mobile computing. Additional information is available at www.facebook.com/groups/mag.lsu.

CCT and LA-SiGMA Host Programming Challenge 4 Girls

The Programming Challenge 4 Girls is an international one-day event to introduce ninth and tenth grade girls to programming. CCT and the Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA) sponsored the challenge at LSU on December 7, 2013. LSU became the first university in the United States to host the challenge.

Twenty girls came to campus to attend this free event designed to be approachable, fun, educational, and challenging. They were engaged in computer science and introduced to female undergraduate and graduate students in science, technology, engineering, and math (STEM) disciplines. The event was a fun-filled chance to learn computer programming through storytelling and get the girls excited about STEM before they make their senior high school subject choices.

Working in teams of two, the girls were able to learn the programming language Alice. Alice is used because it is 3D and colorful, easy to learn, educational, engaging, fun to work with, and has multiple degrees of challenges.

CCT Hosts ACM International Collegiate Programming Contest – South Central Region

CCT was one of three hosts for the south central region of the Association for Computing Machinery (ACM) International Collegiate Programming Contest (ICPC) on November 1-2, 2013. Other south central region host sites were Baylor University (where ICPC is headquartered) and LeTourneau University in Longview, Texas.

The contest was a chance for each of the contestants – working in teams of three – to test their skills at comprehension, analysis, problem solving, coding, debugging, resource management, self-control, and communication. Of the 59 teams in the region, 13 teams from across the state competed at the LSU site.

The winner of the south central region, the University of Texas at Brownsville team – the Ocelots – advanced to the 2014 International Programming Contest.

ICPC is the premiere global programming competition conducted by and for the world's universities. The competition operates under the auspices of ACM and is sponsored by IBM. For nearly four decades, the ICPC has grown to be a game changing global competitive educational program that has raised aspirations and performance for generations of the world's problem solvers in the computing sciences and engineering.

CCT Hosts Fifth Annual SCALA Meeting

Since 2009, the Center for Computation & Technology (CCT) and Tulane University's Center for Computational Science co-sponsored the **Scientific Computing Around Louisiana**, or SCALA, workshop. The workshop focuses on cutting-edge topics in scientific computing, or using computers to examine and solve scientific problems through the analysis of mathematical models. Louisiana State University and Tulane alternate hosting the workshop on their campuses. In February 2014 the workshop was held in the Louisiana Digital Media Center, CCT's new home.

Invited speakers were **Pavel Bochev** of the Sandia National Laboratory; **Yi Jiang** of Georgia State University; and **Tim Warburton** of Rice University.

The workshop showcased the exciting research under way at Louisiana colleges and universities and helped to foster collaborations across the state.

SCALA was founded and is organized by **Susanne C. Brenner**, Michael F. and Roberta Nesbit McDonald Professor of Mathematics and CCT Core Computational Science focus area lead, and Lisa Fauci, Pendergraft Nola Lee Haynes Professor of Mathematics at Tulane.

The sixth annual SCALA workshop will take place at Tulane on March 20-21, 2015.

Red Stick FutureFest at the Louisiana Digital Media Center

More than 300 people attended the 2014 Red Stick FutureFest showcasing LSU projects forging innovative uses of technology and featuring the Center for Computation & Technology's (CCT) Cultural Computing focus area on May 9 at the Louisiana Digital Media Center (LDMC). More than 40 exhibits were on display during the three-hour exhibition, and every half-hour showcases called FutureCasts were held in the LDMC state-of-the-art theater.

The festival is a revitalization of the International Red Stick Animation Festival, which will mark its 10th anniversary in 2015. The broader FutureFest has transitioned to digital art, encompassed by cultural computing, which includes animation, movies, scientific visualization, and games. The festival serves as a hub for ideas, information, innovation, and inspiration; it presented a sampling of digital research and culture.

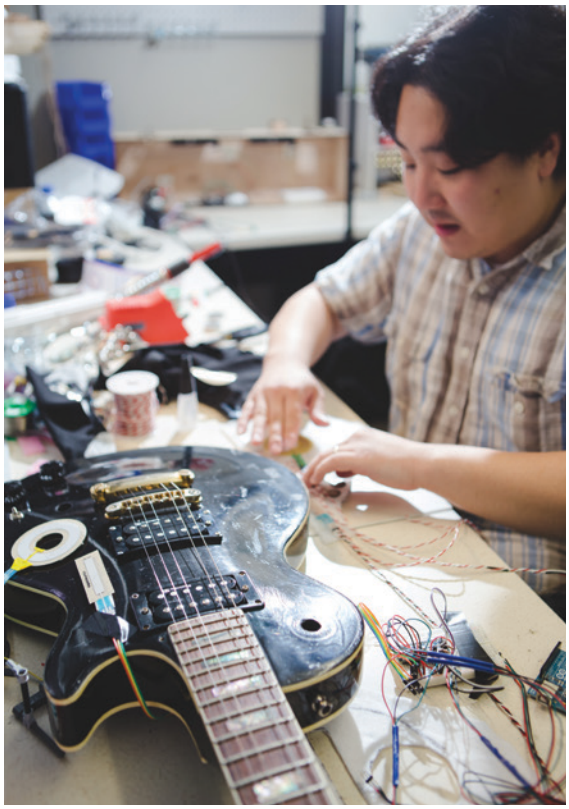
Louisiana has invested time, money, and effort into digital media as an identity for the state. Already it has inspired rapid economic development, strong corporate investment and entrepreneurship, as well as remarkable advances in the digital culture in the state. The Red Stick FutureFest serves as a way to expose a larger audience to the emerging digital culture and tech advances.

CCT's **Jesse Allison** spearheaded the 2014 FutureFest. One of the pieces of art on exhibit was Humming Mississippi, the result of collaboration between Allison and CCT's **Derick Ostrenko** (see sidebar). Another exhibit featured was ORIGIN, an EnOvation project led by **Nick Erickson** of the LSU Department of Theatre, in collaboration with civil engineering and experimental music departments that was performed at the international Edinburgh Festival Fringe in July.

Next year's Red Stick FutureFest will be May 29-31, leading up to the 2015 New Interfaces for Musical Expression (NIME) conference scheduled May 31-June 3. Previous host cities of this prestigious international conference include Seoul and London.

"It's huge that the NIME will be in Baton Rouge," Allison said. "CCT is a big reason why it's coming here. It brings together musicians and technologists to present research, interact with sound, exhibits, and a crazy, eclectic set of things."

The 2015 Red Stick FutureFest is an open source festival – a Louisiana festival built from the contributions of those whose interests and passions are at the point where technology and society meet. The call for participation is open at http://redstickfestival.org, and organizers are looking for event and program ideas that celebrate science, technology, engineering, art, and math.



Danny Holmes

Photo by Josh Hall

Humming Mississippi

Photo by Josh Hall

Humming Mississippi is a sonic sculpture created by CCT's **Derick Ostrenko** and **Jesse Allison** that transforms a linear reading of the Mississippi River's topology combined with a sonification of real-time river data including temperature, salt content, flow rate, and river height into an interactive organic art exhibit.

A mobile application allows viewers to interact with the piece by manipulating the pitch of sonic hums that play back through their device and the installation in real-time. The performance is presented on 18 cedar planks that represent 18 miles of the riverbed. Small transducers attached to the back of each board transform the planks into speakers colored by the individual characteristics of the wood and influenced by the carving of the river's contours.

Ostrenko has a joint appointment with the LSU School of Art, and Allison has a joint appointment with the LSU School of Music. They collaborated with the Louisiana State University's Coastal Hydraulics Lab to create Humming Mississippi. The lab provided a Light Detection and Ranging (LIDAR) scan of the Mississippi River floor that was used to create the 18 planks.

Individuals can interact with the exhibit by visiting http://hummingmississippi.net or by using a mobile application. Viewers can manipulate the pitch of sonic hums that play back through their device, other users' devices, and the installation in real-time.

Humming Mississippi debuted at the LSU Museum of Art as part of the Right Here, Now exhibition in 2013, displayed at the 2014 Red Stick FutureFest in Baton Rouge in May, and was shown at the New Interfaces for Musical Expression conference in London in June and July 2014. Next it will be installed for the International Symposium of Electronic Arts at the New York University galleries in Abu Dhabi, United Arab Emirates, in November 2014. A permanent home for the piece is still in the works.

CYBERINFRASTRUCTURE

SuperMIC: One of America's Fastest Supercomputers

LSU's newest supercomputer SuperMIC (pronounced as Super Mick) has come online this year and was ranked **fifth** fastest among supercomputers at **academic institutions in the United States** as of June 2014. It was funded by a $3.92 million National Science Foundation (NSF) Major Research Instrumentation (MRI) award to the Center for Computation & Technology (CCT) in September 2013; CCT and the Office of Research and Economic Development at LSU provided an additional $1.68 million as match.

SuperMIC is the 65th most powerful supercomputer in the world, according to Top500.org, a site that ranks supercomputers. Rankings are made using the LINPACK Benchmark, which evaluates the machines' performance by providing a dense system of linear equations to solve.

In this year's Top500 list, SuperMIC's performance achieved 557 TeraFLOPS. In context, 1 TeraFLOPS is equal to one trillion floating-point operations per second or one trillion FLOPS.

SuperMIC is being harnessed for a variety of research projects

involving discovery of new drugs, modeling coastal processes, and forecasting hurricane-generated waves and storm surges. The new computing cluster is the next step in supercomputing for Louisiana and allows LSU to better prepare students and faculty for the next generation of high-performance supercomputers.

Housed in the LSU Frey Computing Services Center machine room, SuperMIC is the first of its kind in Louisiana. Hundreds of scientists throughout the state are able to use the supercomputer for research projects requiring processing of large amounts of data.

Scientists from outside Louisiana can use SuperMIC through the Extreme Science and Engineering Discovery Environment (XSEDE), a virtual system supported by the National Science Foundation that scientists use to interactively share computing resources, data, and expertise. The supercomputer is open for LSU and XSEDE users, with 40% of its computational resources reserved for XSEDE participants.

In addition to research use, SuperMIC supports education projects throughout the state, including the CCT and Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA) research experiences for undergraduates (REU) programs, boot camps to introduce high-school students to supercomputing and distance-learning classes.

SuperMIC's total computing capacity or processing speed is 1 PetaFLOPS (or 1000 TeraFLOPS), equivalent to one quadrillion operations per second. For comparison, the fastest supercomputer in the United States (no. 2 in the world), Titan at the Oak Ridge National Laboratory, is capable of 27 PetaFLOPS.

Board of Regents' Latest Supercomputer for Louisiana: Queen Bee 2

Louisiana's latest supercomputer to come online is Queen Bee 2 (QB2), which is 1.5 times faster than Louisiana State University's SuperMIC. Funded by the Louisiana Board of Regents through the Louisiana Optical Network Initiative (LONI), QB2 replaces the state's aged flagship supercomputing system, Queen Bee. QB2 will be available to researchers across the state in November 2014.

Queen Bee has been in production service for the state research community since 2008. Half of Queen Bee's computational cycles were contributed to support the national research community in exchange for $3.8 million in National Science Foundation (NSF) funding to LSU/LONI in February 2008 through March 2012 for user support and system operations. The NSF funding enabled Queen Bee to be added to the national TeraGrid network and its successor named Extreme Science and Engineering Discovery Environment (XSEDE). LSU's Center for Computation & Technology (CCT), a LONI partner, spearheaded the Queen Bee project.

High Performance Computing at LSU (HPC@LSU), a joint partnership between CCT and LSU's Information Technology Services (ITS), operates

all the LSU/LONI clusters and provides services to the research community at all LONI-connected campuses.

The Board of Regents' $6.7 million QB2 system is equipped with 480 NVIDIA graphical processing unit (GPU) compute nodes, 16 Intel Xeon Phi compute nodes, four visualization compute nodes, four big memory compute nodes, 1 GPU head node, 1 Xeon Phi head node, 1 network file system server node, 2 cluster management nodes, 1600 TB Lustre storage, and a FDR (Fourteen Data Rate) InfiniBand.

Housed in the State Information Services Building (ISB) in downtown Baton Rouge, Its peak capacity is 1.5 PetaFLOPS or one quadrillion floating point operations per second (FLOPS). QB2 has already reached 71% efficiency during its commissioning phase. QB2 is expected to be listed among the top 50 machines when TOP500's list of the fastest supercomputers in the world is released at the SC14 Conference later in November.

The QB2 computer architecture was designed with the input of faculty from six major universities in the state: Louisiana Tech, University of New Orleans, University of Louisiana–Lafayette, Tulane University, LSU, and Southern University. QB2 is a statewide project, and researchers across the state can use QB2 through LONI.

LONI is a state-of-the-art fiber optics network that runs throughout Louisiana and connects Louisiana and Mississippi research universities to one another as well as to Internet2. LONI provides Louisiana researchers with one of the most advanced optical networks in the country and the most powerful distributed supercomputer resources available to any academic community. Additional information may be found online at www.loni.org.

CCT Named Intel Parallel Computing Center

Through a grant from the Intel Corporation, the Center for Computation & Technology (CCT) will work to develop open source software focused on simulation of flows through micropores, such as those found in rocks involved in oil and gas extraction. CCT was named an **Intel Parallel Computing Center** (IPCC) in March 2014.

The LSU IPCC will work to scale, optimize, and profile the performance of OpenFOAM, popular open source simulation software, running on Intel Xeon Phi coprocessors such as those installed in SuperMIC, LSU's newest high-performance computing, (HPC) cluster (see page 42). The work will help in developing algorithms suited to fundamental physics problems that use HPC resources efficiently. Since open source community codes will be used, the enhancements will become generally available to the user community.

"At CCT, we use HPC to unite experts in numerous fields of study," said **Honggao Liu**, CCT deputy director and the leading principal investigator for the project. "This grant and multi-disciplinary project will allow us to better understand and solve issues within this critical software. Working with Intel not only benefits LSU by giving us access to Intel's vast expertise, but it also benefits each of the departments involved in the project as well as those who will be able to use the enhancements we work to develop."

In becoming an IPCC, LSU joined other prestigious universities including the Georgia Institute of Technology, Purdue University, the University of Tennessee, and the University of Texas at Austin's Texas Advanced Computing Center, among others.

"Modernizing the underlying codes used in scientific and industrial research is critical to advancing the pace of discovery and innovation," said **Bob Burroughs**, the director of technical computing ecosystem enabling at Intel. "We're thrilled to have LSU join us in this effort. The work they'll accomplish on modernizing OpenFOAM codes for Intel architecture will have a broad and lasting impact on the community for years to come."

In addition to Liu, other principal investigators on the project are **James A. Lupo**, CCT assistant director for computational enablement; **Mayank Tyagi**, recipient of the Adolphe G. Gueymard professorship in the Craft & Hawkins Department of Petroleum Engineering and CCT; **Krishnaswamy Nandakumar**, Gordon A. and Mary Cain Endowed Chair Professor in the Cain Department of Chemical Engineering and CCT adjunct faculty member; and Karsten Thompson, chair of the Craft & Hawkins Department of Petroleum Engineering.

The broader computational sciences community will benefit greatly from the distribution of accelerated modules of OpenFOAM, which may lead to improvements in other computational fluid dynamics-related projects.

"OpenFOAM development on the latest accelerator technology from Intel is of great value to scientists and engineers. CCT and LSU greatly value our partnership with Intel," said CCT Director **J. "Ram" Ramanujam**.

About Intel Parallel Computing Centers

Intel Parallel Computing Centers are universities, institutions, and labs that are leaders in their field. The centers are focusing on modernizing applications to increase parallelism and scalability through optimizations that leverage cores, caches, threads, and vector capabilities of microprocessors and coprocessors. Code modernization is expected to enable large performance increases while maintaining the code portability users expect. Training engineers on modernizing their code is also necessary. To meet this need, the centers are developing a curriculum to equip students, scientists, partners, and computer scientists with the skills to fully realize the capabilities of parallel computing resources. By enabling the advancement of parallelism, the Intel Parallel Computing Centers will accelerate discovery in the fields of energy, finance, manufacturing, life sciences, weather, and beyond.

ECONOMIC DEVELOPMENT

Louisiana Digital Media Center Formally Dedicated, Home to CCT and Electronic Arts Inc.

Photo by University Relations

The new, $29.3 million Louisiana Digital Media Center (LDMC) was formally dedicated on February 10, 2014. Governor **Bobby Jindal**, Electronic Arts Inc. (EA) executive **Bryan Neider**, and LSU President and Chancellor **F. King Alexander** formally dedicated the 94,000 square foot technology hub. It serves at the permanent home of the Electronic Arts' North American Test Center and the LSU Center for Computation and Technology (CCT).

"LSU is proud to be a partner in the Digital Media Center and the perfect marriage between education and industry it represents," Alexander said at the dedication. "I believe we're all aware of how important the digital media industry is to our state and how fast it is growing. At LSU, we're proud to supply solutions to these training and workforce demands while also contributing technological advancements and computational needs for the digital media industry."

Located on the southeast corner of LSU's campus, the three-story LDMC provides a permanent, contemporary facility for CCT to house programs that accelerate academic and industry research in an innovative environment. The center is filled with technological perks, including state-of-the-art cinema sound system and top-of-the-line digital video projector in the theater and a high-quality recording studio. The Digital Media Arts & Engineering program at LSU occasionally presents free film screenings and Cinema for the Ears Concerts in the center's theater. Faculty and staff moved into the new building in August 2013.

Photo by University Relations

"The LDMC represents an important milestone for the university and especially for the Center for Computation & Technology," **Stephen Beck**, former CCT director and current LSU School of Music director, said at the dedication. "The new building provides state-of-the-art labs and research spaces for our faculty and finally brings us all together under one roof. It creates and encourages the collaboration among our diverse groups, and the new computing resources will enable the development of next-generation computer and media technologies."

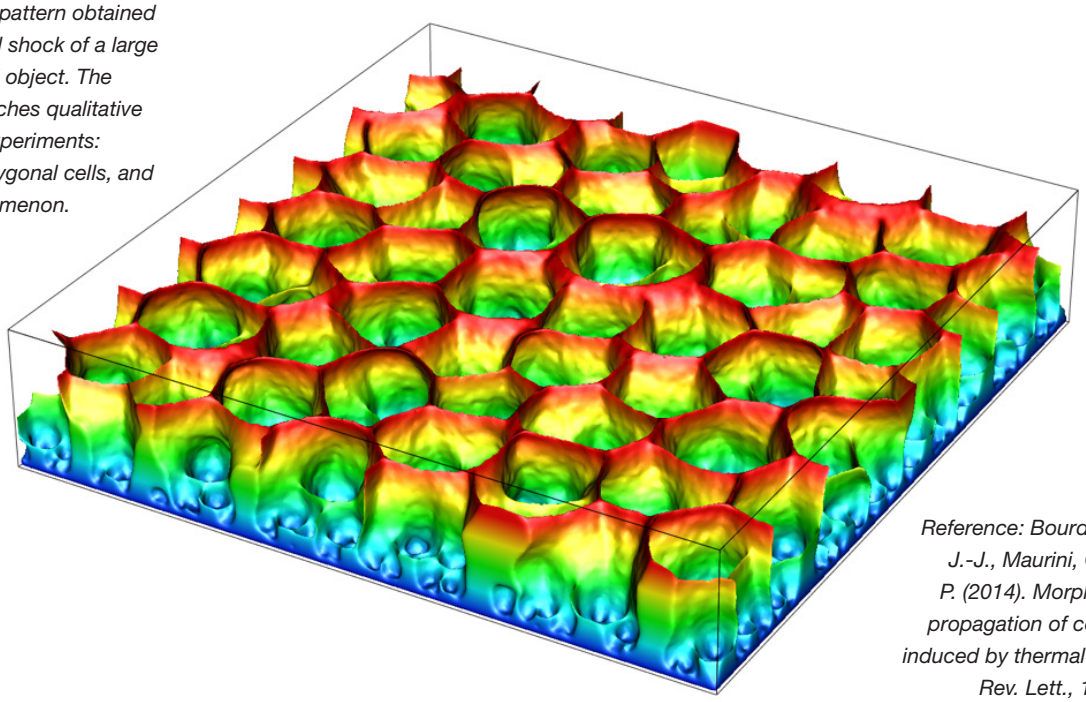
State, local, federal, and EA company leaders broke ground on the center in mid-2011, and its dedication fulfilled a collaborative vision to house EA's commercial video game operations in the same building with CCT's high-performance computing research and the university's digital media initiative, Arts, Visualization, Advanced Technologies & Research (AVATAR).

AVATAR unites faculty from many disciplines and enables students to conduct research and complete projects in virtual environments, digital art, electro-acoustic music, animation, video game design, and scientific visualization. More than 200 students use the facilities and classrooms each week. More than 600 people work in the building for CCT and EA.

The state funded the center in connection with its 2008 recruitment of EA to Baton Rouge. Construction of the center was funded primarily by $26.3 million of state capital outlays and a $3 million infrastructure grant from the U.S. Economic Development Administration.

From Theory to Application: Forming Industry Research Partnerships

Complex fracture pattern obtained during the thermal shock of a large three-dimensional object. The crack pattern matches qualitative observations in experiments: emergence of polygonal cells, and coarsening phenomenon.



Reference: Bourdin, B., Marigo, J.-J., Maurini, C., and Sicsic, P. (2014). Morphogenesis and propagation of complex cracks induced by thermal shocks. Phys. Rev. Lett., 112(1):014301.

Developing partnerships with industry and balancing academic and applied research is something **Blaise Bourdin** knows well. An LSU math professor and adjunct faculty member in the Center for Computation & Technology (CCT), Bourdin has worked to keep an eye toward industry collaborations when seeking federal research support.

For example, his 2008 grant from the National Science Foundation to study geothermal energy led to a partnership with Chevron. Within two years the federally funded, theoretical research had become industry-funded and applied research – a very fast timeline.

"Although this type of applied, industry-funded research is sometimes less publishable it is very good training for students who are ready to work," Bourdin said. **Chukwudi Chukwudozie**, a Ph.D. student at LSU, is supported by the Chevron project and works on combined flow and fracturing layer.

Another good example of industry partnerships is Bourdin's recent agreement with Corning to work on fundamental fracture mechanics. While the company has amazing research teams and thinks long-term in its strategic research, industry can't compete with academia for theoretical research.

Bourdin favors leveraging academic deep and broad knowledge over commercializing university assets as an approach to industry–academia collaboration.

"We need to do what we're good at, which is solving broad problems," Bourdin said. "And CCT is fantastic for that because we know each other, how to talk to each other, and know who knows what. It's a special combination of breadth and ability to solve problems – something you won't find in industry."

Bourdin's partnership with Chevron continues, and the next part of the project is working on the theoretical mechanics of solids. In collaboration with **Jean-Jacques Marigo** at École Polytechnique (France) and Ph.D. student **Enwan Tanné**, Bourdin is trying to gain both a deeper understanding of the mechanism of failure in rocks and improve the accuracy of classical techniques used by the industry for measuring fracture properties of rocks.

"A better knowledge of challenges facing industry can suggest new fundamental research directions in academia," Bourdin said. "Industry benefits from better theoretical understanding as well."

A Case for an Industrial Commons in Chemicals and Energy Sector Along the Mississippi River

By **Krishnaswamy "Kumar" Nandakumar**, Gordon A. and Mary Cain Endowed Chair Professor in the Cain Department of Chemical Engineering and CCT adjunct professor, and **Mayank Tyagi**, Adolphe G. Gueymard associate professor in the Craft & Hawkins Department of Petroleum Engineering and CCT

A new consortium at Louisiana State University called Enabling Process Innovation through Computation (EPIC) aims to synergistically connect faculty research and engineering graduate training with the needs of chemical and energy industry to address challenges in the design of next generation process plants that will progressively use hybrid feed stocks (fossil and bio based) and must be designed to be environmentally benign and energy efficient.

The consortium will concurrently meet the workforce development needs of a buoyant economy in Louisiana and train the graduates to be process *innovators* employed in a range of industries that are engaged in *engineered manufacturing process systems* from energy production, environmental remediation, chemical and advanced materials manufacturing operations.

The EPIC consortium will advance the fundamental science of multiphase flows that governs many of these *engineered process systems*. EPIC will *shift the design paradigm* of such processes from a largely empirical approach (as currently practiced) to one that makes full use of advances in computational, experimental and manufacturing technologies. In particular, the consortium will focus on investigation of multiphase transport in process systems in the presence of large scale heterogeneities and to manage such heterogeneities right from the conceptual design stage of the equipment itself.

EPIC will be developing *experimentally validated high fidelity computational models* that enable exploration of a large design space in a cost effective manner. EPIC, with well-conceived research agenda coupled with industrially relevant test-beds for proof of concept, will converge technologies in High Performance Computing (HPC), high fidelity measurements (tomography, PIV), and high precision, complex manufacturing. Such convergence enables study of large complex design spaces on all scales, making possible new process designs.

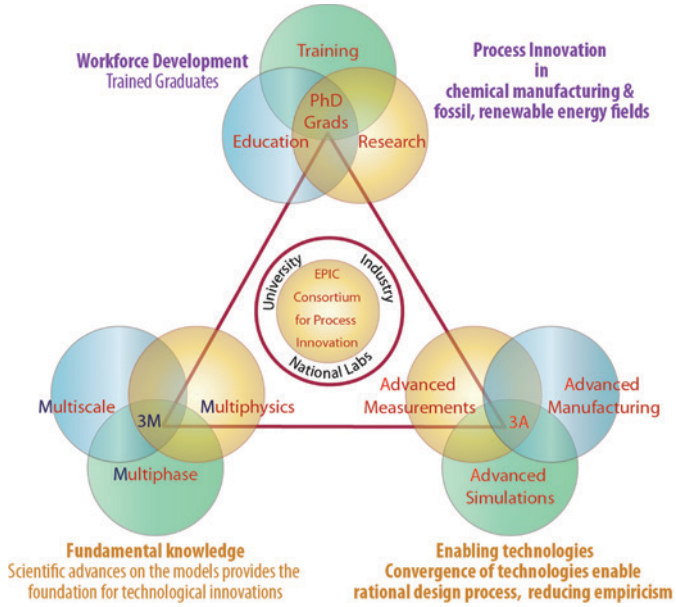
The synergy between faculty expertise at LSU and partner universities, the advanced infrastructure offered by the Center for Computation & Technology (CCT) in computing, Center for Advanced Microstructures and Devices (CAMD) in high fidelity measurements, and the opportunity to engage nearly 300 local companies along the Mississippi River provide an ideal environment for an *industrial commons* in this space centered on Baton Rouge.

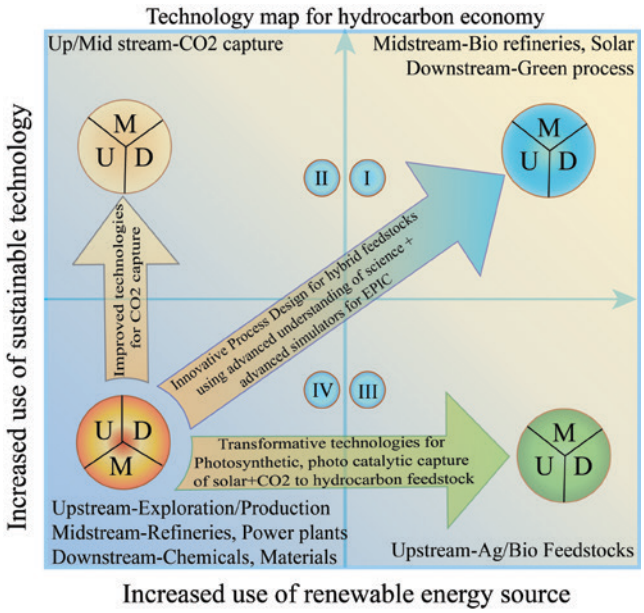
AN OPPORTUNITY FOR INNOVATIONS IN CHEMICALS MANUFACTURING

Rapid globalization of businesses, volatility in energy prices, availability of shale resources, and emergence of low cost labor markets have changed the landscape of traditional chemical manufacturing and petroleum refining industries dramatically. In a recent address by Stephen Pryor, president of ExxonMobil Chemical Company, on "Innovation and the Evolution of Chemical Feedstocks," he singled out the *boom in shale gas and liquids* in North America as being the most dominant factor and a game changer that is revolutionizing the global chemical and petrochemical industries by evolving their advantaged feedstocks. American manufacturers use natural gas to fuel and power a wide variety of processes to produce a broad portfolio of manufactured goods – from a variety of performance monomers, specialty chemicals, pharmaceuticals, advanced materials agrochemicals and cosmetic consumer products. Although low cost energy sources provide an immediate advantage, it may not be as sustainable as those advantages achieved by sustained innovations.

A CASE FOR LOUISIANA INDUSTRIAL COMMONS

Louisiana has traditionally played an important role in the chemical and petrochemical industries as well as the upstream petroleum exploration and production. A report titled "The Economic Impact of the Chemical Industry on the Louisiana





Left: Schematic of a collaborative consortium involving universities, industries, and national laboratories in the area of process innovation in the chemical manufacturing and energy industries.

Right: Technology roadmap for innovation in chemical processing industries.

Economy," notes that chemicals are Louisiana's third largest export, shipping $8.3 billion (14.4 percent of total production in the state) in chemical products to other parts of the world in 2011. Petroleum and agricultural products are No. 1 and No. 2. Chemicals are the No. 1 producer of direct jobs in Louisiana's manufacturing sector (26,944 people in 2011). Louisiana ranked No. 3 among the 50 states in terms of the total value of chemical shipments (~$58.2 billion in 2010). With 19 operating refineries, Louisiana was second only to Texas in 2013 in both total and operating refinery capacity. The Louisiana Offshore Oil Port is the only port in the United States capable of offloading deep draft tankers. The U.S. Strategic Petroleum Reserve's two Louisiana facilities consist of 29 salt caverns capable of holding more than 300 million barrels of crude oil. In 2011, Louisiana ranked second among the states in total energy consumption per capita, primarily because of the industrial sector (about 2/3rds of consumption), which includes many refineries and petrochemical plants, according to the U.S. Energy Information Administration at www.eia.gov.

To understand the role of universities in this landscape, an NRC study titled, "International Benchmarking of U.S. Chemical Engineering Research Competitiveness" points out *"Future U.S. leadership in chemical engineering is not guaranteed. Many factors could significantly affect the position of the U.S., and these include shifting funding priorities by federal agencies, reductions in industrial support of academic research in the United States, and decreases in talented foreign graduate students, among others."* This report points to an urgent need for rejuvenating research and training elements focused on *process innovation* to maintain U.S. competitiveness in this sector.

TECHNOLOGY ROADMAP

The accompanying technology road map envisions two metrics, one on the use of renewable energy sources and another on sustainable technology development. This divides the hydrocarbon-based economy into four quadrants and the current economy is on the 4th lower-left quadrant where reliance is on fossil fuel and the environmental sustainability takes a back seat. By incorporating hybrid feedstocks (i.e. increased dependence on renewable feedstocks), we move to the right (quadrant 3), and by adopting carbon sequestration (i.e. reduced emissions and improved environmental sustainability) we move to quadrant 2. A combination of these is needed to move to the ideal quadrant one. The EPIC consortium can assist in

Mississippi River chemical corridor shown by the locations of various chemical products at geographically distributed plants along the river. (Petrochemical America; Aperture 2012 © SCAPE)

this transformation by introducing process innovations that adopt hybrid feedstocks and account for reduced environmental impacts during the design process itself. Such technologies are the outcomes of a sustained innovation cycle that involves all potential stakeholders including both the technology developers and the end users during the research and testing stages.

The figure on the right shows the interactions necessary among fundamental knowledge (university engagement), enabling technologies, and innovative test beds (industry engagement).

LSU AS THE STRATEGIC PARTNER

LSU has excellent high-performance computing facilities (SuperMIC is 65th among top 500 facilities in the world as of June 2014, see page 42), and advanced computational modelling is a key aspect in the road map. CAMD and advanced synchrotron, tomography, based measurement capabilities, are unique to this region. Advanced simulator development to model such complex processes as hydraulic fracturing, bioreactor development, geothermal energy development will move us from quadrant 4 toward quadrant 1 in the road map. Additional expertise in heat and mass transfer, reactor design, thermodynamics, flow through porous media, etc. will be added as the consortium grows in size on the industrial side, through a series of strategic partnership development with other universities such as the University of Florida, Iowa State University, and The Johns Hopkins University. The orchestration of three levels of interaction among the *expert engineering scientist* on the *fundamentals of multiphase flows*, the *simulation expert* on *validated models* and the *industrial liaison expert* (or chief innovation officer) will coordinate the transfer of sound technological designs that are rooted in the fundamentals to industry.

A CALL TO INDUSTRY

Please contact one of the founders to find out how you can support in workforce development at LSU that is relevant to Chemical and Energy process industries and in advancing the field of process design for next generation plants.

A CALL TO LSU FACULTY

If your research interests align with the goals of EPIC consortium please join us in the effort to build an impactful industrial consortium and achieve the dual goal of workforce development and local industrial engagement.

At present EPIC is collaborating with a number of faculty members on different areas. The expanding list of faculty associated with EPIC includes LSU's **Les Butler**, chemistry; **Blaise Bourdin**, mathematics; **Dimitris Nikitopoulos**, mechanical engineering; **Kerry Dooley**, chemical engineering; and **Karsten E. Thompson**, petroleum engineering, and **Daira Aragon Mena**, Audubon Sugar Institute.

Visit the EPIC consortium's website at http://epic.lsu.edu.

LAGNIAPPE

Faculty Promotions

In 2013 and 2014 four CCT assistant professors were promoted to the rank of associate professor with tenure. **Xin Li** and **Georgios Veronis** were promoted in the School of Electrical Engineering & Computer Science, Division of Electrical & Computer Engineering. **Hongchao Zhang** was promoted in the Department of Mathematics, and **Mayank Tyagi** was promoted in the Craft & Hawkins Department of Petroleum Engineering.

In addition, CCT faculty member **Bijaya Karki** was promoted to full professor in the School of Electrical Engineering & Computer Science, Division of Computer Science & Engineering.

CCT adjunct faculty members **Blaise Bourdin** and **Dorel Moldovan** were promoted to full professor, Bourdin in the Department of Mathematics and Moldovan in the Department of Mechanical & Industrial Engineering.

Notable Publications

Michal Brylinksi, assistant professor in the Department of Biological Sciences and CCT, authored "Sequence Order-Independent Structure Alignments of Ligand Binding Pockets in Protein Models," which was featured on the cover of the September 2014 issue of *PLoS Computational Biology*, one of the top journals in computational biology.

Brygg Ullmer, associate professor in the School of Electrical Engineering and Computer Science, Division of Computer Science and Engineering, and CCT Cultural Computing focus area lead, was an author of a *Nature* cover article, "Gibbon genome and the fast karyotype evolution of small apes," published September 11, 2014.

"Quantum Information Theory," a textbook by **Mark M. Wilde**, assistant professor in the Department of Physics & Astronomy and CCT, was published by Cambridge University Press in June 2013. So far, the book is being used for classes at Cambridge, Princeton, Cal Tech, the University of Southern California and LSU.

CCT adjunct faculty member and professor at the LSU School of Art, **Susan Elizabeth Ryan's** book "Garments of Paradise: Wearable Discourse in the Digital Age," was published by MIT Press in June 2014.

New Hires for Fall 2014

Jun-Hong Liang, assistant professor in the Department of Oceanography & Coastal Sciences and CCT, received his master's degree in civil and environmental engineering from Hong Kong University of Science and Technology and his Ph.D. in atmospheric and oceanic sciences from the University of California, Los Angeles.

Celalettin Emre Özdemir, assistant professor in the Department of Civil and Environmental Engineering and CCT, joined LSU from Woods Hole Oceanographic Institution. He received his Ph.D. in civil engineering from the University of Florida, Gainesville.

Gabriele Piccoli, the Edward G. Schlieder Endowed Chair of Information Sciences in the Department of Information Systems & Decision Sciences and faculty at CCT, received his Ph.D. and a Master's of Business Administration from the E.J. Ourso College of Business at LSU. He received a Laurea in Economia e Comercio from the University of Pavia, Pavia (Italy). He was a full professor at Grenoble Ecole de Management (France) and Associate Professor of Information Systems at Cornell University and University of Pavia and subsequently Associate Professor of Applied Economics at the University of Sassari (Italy). His research, teaching, and consulting expertise is in strategic information systems and the use of information systems to enable customer service.

Zuo (**George**) **Xue**, assistant professor in the Department of Oceanography & Coastal Sciences and CCT, received his Ph.D. in marine sciences from North Carolina State University in 2010. His dissertation examined transport and deposition of Mekong River sediment. Before joining LSU, Xue was a research assistant professor at NCSU where his research focused on coupled ocean models.

New Hires for Spring 2015

Scott Charles Hagen received his Ph.D. in civil engineering from the University of Notre Dame in May 1998. Hagen will join as a professor in the Department of Civil and Environmental Engineering and CCT in spring 2015; currently he is a full professor at the University of Central Florida and is a Fellow of the American Society of Civil Engineers (ASCE). He serves on the predictive modeling technical advisory group for the 2017 Louisiana Coastal Master Plan as well as numerous other state and national boards.

Giulio Mariotti received his Ph.D. in coastal geomorphology from Boston University in January 2013 and is currently a W.O. Crosby Postdoctoral Fellow at the Massachusetts Institute of Technology's Department of Earth, Atmospheric, and Planetary Sciences. He will join the Department of Oceanography & Coastal Sciences and CCT in spring 2015.

Three CCT Faculty Members Receive NSF CAREER Grants

The Center for Computation & Technology's **Georgios Veronis**, **Mark M. Wilde**, and **Francisco Hung** have each received five-year National Science Foundation Faculty Early Career Development, or CAREER award. The CAREER award 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.

Veronis, now the Rubicon Distinguished Associate Professor of the LSU Division of Electrical & Computer Engineering and CCT, is receiving support for the development of physics-based modeling techniques, which could lead to novel nanoplasmonic devices with optimal performance and minimum size for high-density optical information processing.

"The realization of such devices would tremendously expand the applicability of plasmonics and would have profound implications for computing and communications," Veronis said.

Veronis' plan consists of developing physics-based models for 3D plasmonic waveguides and devices and using these models to develop optimization techniques of multi-parameter nanoplasmonic devices that greatly reduce the required number of computationally expensive full-wave device simulations. In addition, modeling techniques that calculate the effect of random manufacturing imperfections on nanoplasmonic devices will be developed. These techniques will, in turn, be utilized to design robust nanoplasmonic devices.

"The results of the project will represent important breakthroughs in integrated optics, optical information processing, and renewable energy sources, which have broad impacts on modern technology and human life," Veronis added.

As part of the award, Veronis will develop a new interdisciplinary course, provide research opportunities for undergraduate students, and enhance minority undergraduate research and education opportunities. In addition, through outreach to three local high schools with a strong science curriculum, Veronis will introduce students to the field of nanophotonics to generate excitement for careers in science and technology.

Wilde, assistant professor in the Department of Physics & Astronomy and CCT, is receiving support to examine the theoretical and practical aspects of quantum communication protocols.

"The focus is on quantum information theory, trying to figure out what are the limits on communication dictated by quantum mechanics and if we can come up with schemes to achieve those limits," Wilde said. "Most of the work proposed is theoretical in nature, but some of the threads are practical and may find future application in quantum communication systems."

Wilde will work to prove so-called "strong converse" theorems for various

communications capacities of quantum channels. The quantum information community now understands the communication capacities of several channels well, but what is lacking in some cases is a strong converse theorem. These theorems are conceptually rich, sharpen our understanding of communication capacity, and they also find application in proving the security of particular models of cryptography.

The proposal includes a strong educational component in line with Wilde's vision to establish LSU as a leading center for quantum information research and study. In addition to advising and teaching several graduate students in the quantum science and technologies group at LSU, he has connected his work to high school students. In October 2014 he presented "Quantum Information Entanglement … and All that Jazz" at the LSU Physics Science Saturday program for high school students.

Hung, now associate professor in the LSU Cain Department of Chemical Engineering and adjunct at CCT, is receiving support to perform molecular simulations to fundamentally understand the behavior of phases of ionic liquids (ILs) confined in nanoporous materials.

ILs are organic salts that are in liquid state near room temperature and have been proposed as alternative electrolytes for several energy-related devices such as capacitors, batteries, and solar cells. In addition, inserting and solidifying organic salts inside nanoporous materials is one step in the synthesis of nanomaterials based on organic salts, which have potential applications in sensors, biomedical applications, organic light emitting diodes (OLEDs), energy storage, and CO2 sequestration.

"If successful, the proposed simulation studies will help us understand how the structure of nanoconfined phases of ILs translates into macroscopic properties. This understanding is needed to rationally design IL-based nanomaterials with optimal properties for those applications," Hung said.

The education component of Hung's proposal involves close collaboration with the pre-college programs of the LSU College of Engineering, specifically targeting students in grades 6-12. Due to his Hispanic background, Hung is fully committed to encouraging students from underrepresented minorities to major in STEM programs.

"The proposed studies have the potential to be transformative, taking IL-based nanomaterials from promising lab curiosities to being the first choice in fields like optoelectronics, photovoltaics, sensors, and biomedicine. Our proposed studies also provide opportunities for multiple synergies with our current efforts in graduate and undergraduate research, and outreach and diversity," Hung added.

2013-2014 Honors and Awards

Susanne C. Brenner
- 2013-2014 Distinguished Visiting Professor, Indian Institute of Technology, Bombay
- LSU Distinguished Research Master

Theda M. Daniels-Race
- Michel B. Voorhies Distinguished Professorship #4 in Electrical Engineering

Rudy Hirschheim
- 2013 Best Paper Award, Association for Information Systems, Scholarship/Research, International
- LEO Award for Lifetime Achievement in the Information Systems Field, Association for Information Systems

Xin "Shane" Li
- Oscar R. Menton Professorship in Electrical Engineering

Derick Ostrenko
- 2014 Tiger Athletic Foundation Teaching Award

Seung-Jong Park
- Dr. Fred H. Fenn Memorial Professor

J. Ramanujam
- Floating Point Systems Endowed Chair in Computational Methods

Joel Tohline
- LSU Board of Supervisors has conferred the title of Director Emeritus & Professor Emeritus

Brygg Ullmer
- Effie C. and Donald M. Hardy Professor

Georgios Veronis
- 2013 NSF CAREER Award
- Rubicon Professorship of Engineering, College of Engineering, LSU

Mark Wilde
- 2014 National Science Foundation CAREER Award
- American Physical Society- Indo-US Science and Technology Forum Professorship Award in Physics
- Senior Member of the Institute of Electrical and Electronics Engineers

Hongchao Zhang
- LSU Rainmakers Emerging Scholar Award
- College of Science Faculty Research Award
- LSU Alumni Association Rising Faculty Research Award

ADJUNCT FACULTY:

Dubravko Justic
- 2014 Dean's Outstanding Service Award, LSU School of Coast and Environment
- 2014 CASC brochure cover art competition with W. Benger, I. Ayyala, N. Manya and L. Wang

Daniel Katz
- 2013 Best Paper Award: "Application Skeletons: Encapsulating MTC Application Task Computation and I/O," Proceedings of 6th Workshop on Many-Task Computing on Grids and Supercomputers (MTAGS) (at SC13)
- 2014 Best Paper Award: "Evaluating Storage Systems for Scientific Data in the Cloud," Proceedings of 5th Workshop on Scientific Cloud Computing (ScienceCloud) 2014 , (in conjunction with HPDC'14)

Robert Lipton
- Fellow, American Association for the Advancement of Science (AAAS)

Dorel Moldovan
- 2014 Tiger Athletic Foundation Undergraduate Teaching Award LSU College of Engineering
- Fruehan Family Professor of Mechanical Engineering

Thomas Sterling
- 2013 HPC Vanguard Award

George Voyiadjis
- 2013 Diplome d' Ingenieur Honoris Causa de l' Ecole Polytechnique d' Agadir, Universite Internationale d' Agadir, Universiapolis, Royaume du Maroc

FORMER POSTDOC AT CCT:

Michael Neilan (former postdoc: 2009-2011)
- Leslie Fox Prize in Numerical Analysis (First Prize) 2013
- Sloan Research Fellowship 2014

CCT-Sponsored Conferences and Events Fall 2013 – Summer 2014

Science Visualization Course: August 25-26, 2014

LSU iOS App Boot Camp 2014: August 4-15, 2014

Baton Rouge Energy Venture Camp 2014: July 28-August 1, 2014

Computer Math Summer Camp 2014: July 28-August 1, 2014

Beowulf Boot Camp 2014: July 7-11, 2014

PyFUN Programming Summer Camp 2014: July 21-25, 2014

Gamecrash - Adventures in Game Design Camp 2014: July 14-18, 2014

Girls Rock! - Sound Engineering Camp 2014: June 16-20, 2014

Harness the power of GPUs: Introduction to GPGPU programming: June 16-20, 2014

Alice in Computation Land Summer Camp 2014: June 9-13, 2014

GPU Workshop presented by Nvidia: June 6, 2014

High Performance Computing User Symposium: June 4-5, 2014

LONI Parallel Programming Workshop: June 2-4, 2014

CCT and LaSiGMA Research Experience for Undergraduates: May 26 – August 1, 2014

LaSiGMA Research Experience for Teachers: May 26 – August 1, 2014

LaSiGMA Research Experience for High School Students: May 26 – July 3, 2014

2nd Annual LA Conference on Bioinformatics: May 15-16, 2014

RedStick FutureFest: May 9, 2014

Black Arts Film Festival: April 24, 2014

PAX East Boston, Booth #299: April 11-13, 2014

Cinema for the Ears Concert: April 7, 2014

NanoDays at Highland Road Park Observatory!: April 5, 2014

New Orleans Mini Maker Faire: April 5, 2014

Workshop for Chemical & Energy Industries in Louisiana: April 3, 2014

Intel Xeon Phi Coprocessor Developer Training: April 1, 2014

Mardi Gras Conference 2014: February 27 - March 1, 2014

IBM-LSU Big Data Summit: February 26, 2014

Scientific Computing Around Louisiana Workshop (SCALA): February 21-22, 2014

Global Game Jam @ Louisiana State University: January 24-26, 2014

Programming Challenge for Girls 2013: December 7, 2013

SuperComputing (SC13): LSU Booth #1901: November 18-21, 2013

Laptop Orchestra of Louisiana in Concert: November 11, 2013

ACM ICPC South Central USA Regional Programming Contest 2013: November 1-2, 2013

Training: Introduction to Python Programming: October 23, 2013

Training: Introduction to Perl: October 16, 2013

Semantic Sabotage Workshop: October 15, 2013

Shell Scripting II: October 2, 2013

Shell Scripting I: September 25, 2013

HPC User Environment, Job Management with PBS/Loadleveler Training: September 18, 2013

Introduction to Linux: September 11, 2013

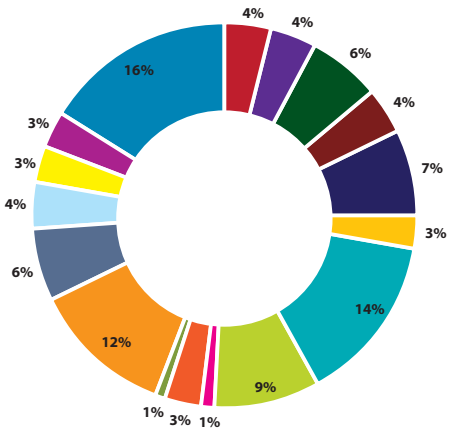
Microsoft Coding Challenge: September 10, 2014

Introduction to High Performance Computing, Accounts and Allocations: September 4, 2013

Microsoft Recruiting: September 3, 2014

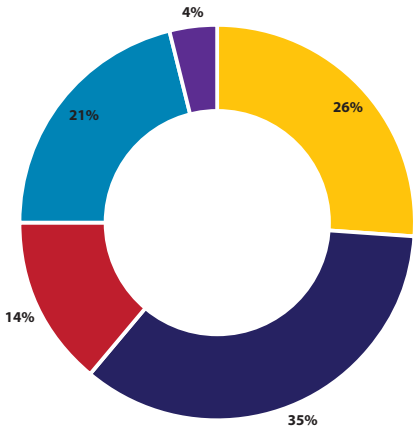
Business Reports

CCT Faculty by Department for FY 2014 (includes adjunct faculty)



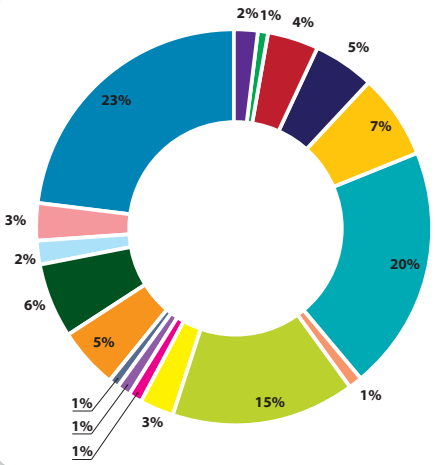
- Chemical Engineering 4%
- Biology 4%
- Mechanical Engineering 6%
- Art & Design 4%
- Chemistry 7%
- Civil & Enviromental Engineering 3%
- Computer Science 14%
- Electrical & Computer Engineering 9%
- Geology & Geophysics 1%
- Information Systems and Decision Science 3%
- Mass Communication 1%
- Mathematics 12%
- CCT 6%
- Music 4%
- Oceanography and Coastal Studies 3%
- Petroleum Engineering 3%
- Physics & Astronomy 16%

CCT Professional Staff for FY 2014



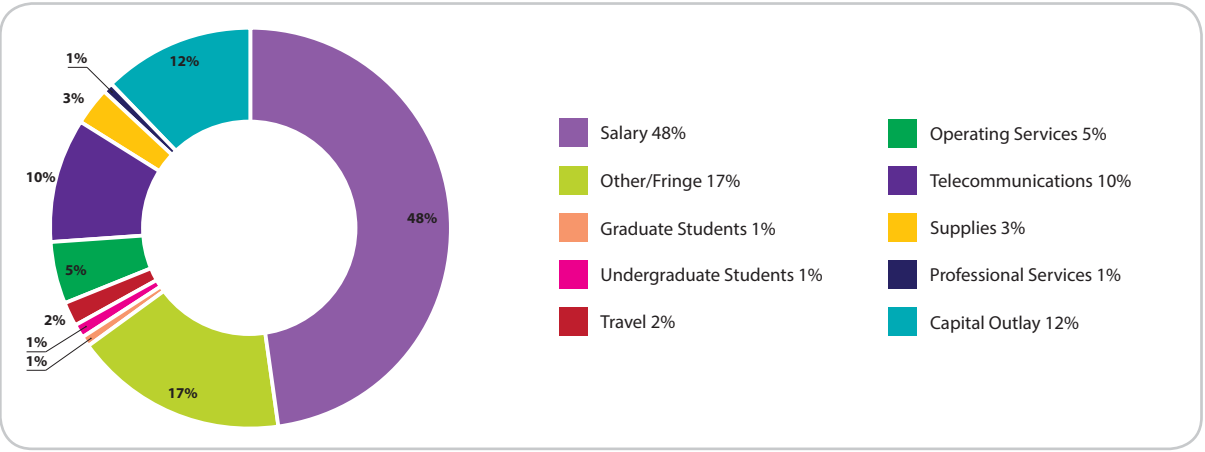
- Research Scientist 26%
- Postdoctoral Researchers 35%
- Technical 14%
- Executive & Administrative Staff 21%
- Economic Development & Digital Media Staff 4%

CCT Graduate Assistants by Department for FY 2014

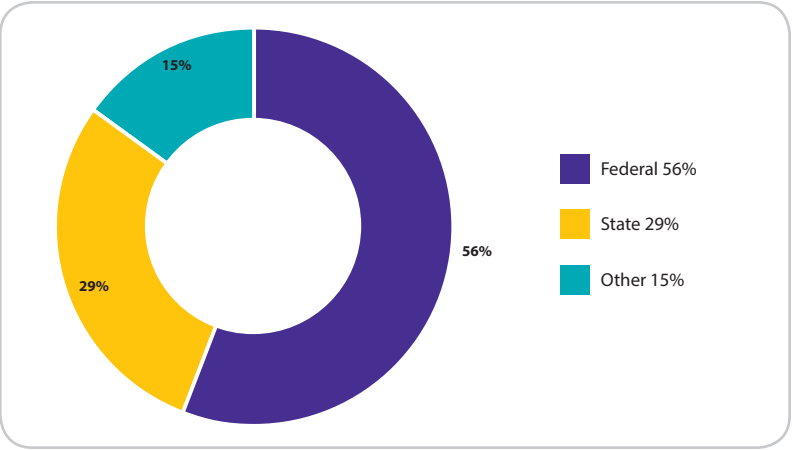


- Biology 2%
- Business 1%
- Chemical Engineering 4%
- Chemistry 5%
- Civil & Enviromental Engineering 7%
- Computer Science 20%
- History 1%
- Electrical & Computer Engineering 15%
- Oceanography & Coastal Studies 3%
- Geology & Geophysics 1%
- Library & Information Sciences 1%
- Education 1%
- Mathematics 5%
- Mechanical & Industrial Engineering 6%
- Music 2%
- English 3%
- Physics & Astronomy 23%

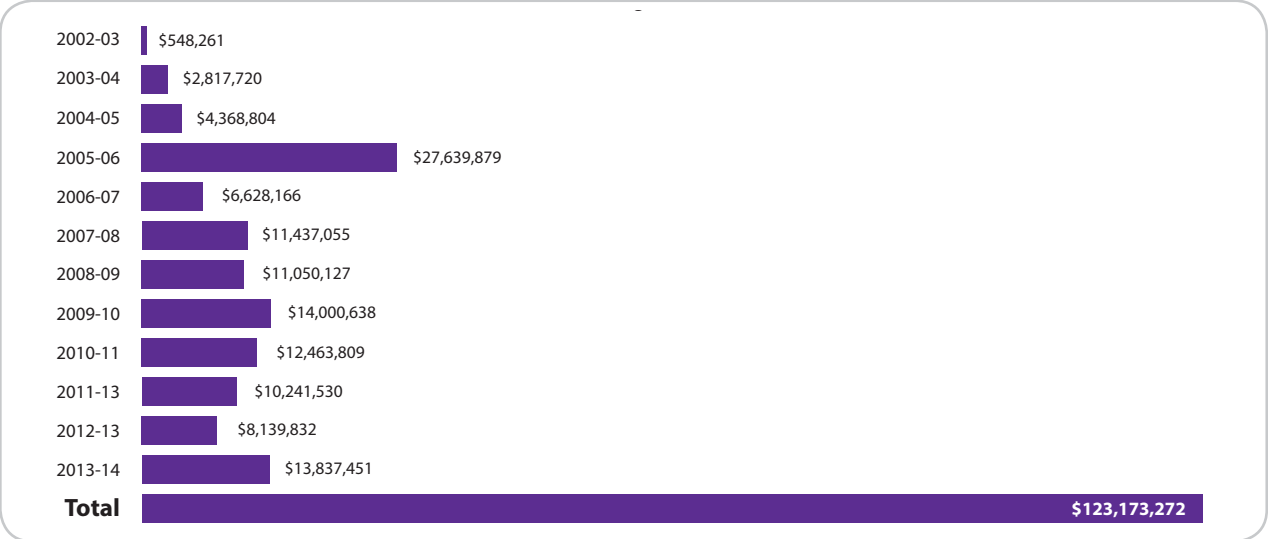
CCT Investment Summary 2013-14



Total External Funding by Source



External Funding FY 2003-2014



LSU