

The image features a complex 3D molecular model of a protein structure. The protein backbone is represented by a ribbon diagram, with different regions colored in shades of purple and yellow-green. A small molecule ligand is bound within the protein's active site, shown as a stick model with atoms colored in red, green, and blue. The background is dark with a faint grid pattern.

COMPONENTS

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Special thanks to Randy Dannenberg,

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Cover Image: Drug discovery is the process by which new pharmaceuticals are developed.

Pharmacological effects are mediated by interactions between drugs and biological macromolecules, proteins in most cases. Although drugs are typically developed to modulate the function of specific proteins, protein-drug interactions are rather promiscuous and the majority of pharmaceuticals exhibit activity against multiple, often unrelated targets. For instance, the cover image shows the superposition of histamine N-methyltransferase (purple) and ATP-dependent DNA ligase (gold) that bind compounds containing the adenosine moiety (shown in the middle). The Computational Systems Biology Group @ LSU developed a suite of computer programs to detect those binding sites having the capability to bind similar drugs. Their approach opens up the possibility to investigate drug-protein interactions at the systems level with prospective applications in polypharmacology and rational drug repositioning. See page 20 for more about drug discovery.

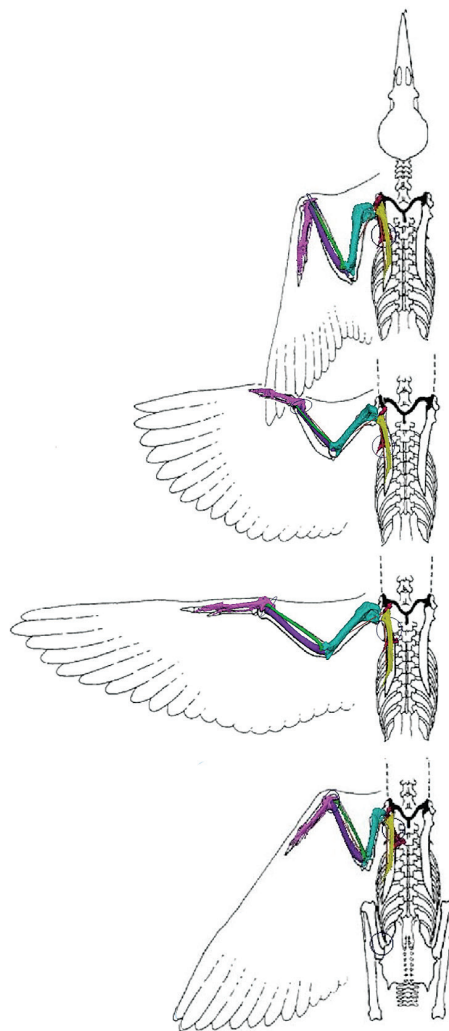
Right: This was a project by 3D Imaging and Animation (HNRS3035) class student Christina Daigle. This honors class was taught by Dominique G. Homberger (Dept. of Biological Sciences) and Jinghua Ge (CCT) in Spring 2016. They will teach this course again in Spring 2017.

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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.



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Message from the LSU Office of Research & Economic Development

The Office of Research & Economic Development's significant efforts toward developing a strategic approach to LSU'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 seven 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 highly multidisciplinary, cross-campus and statewide research activities while developing new partnerships and simultaneously strengthening LSU's existing international partnerships in Asia, South America, Europe and elsewhere. These efforts among other initiatives including increased biomedical and biotechnical research, new big data, analytics and deep learning 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 level. Supercomputing, high performance computing, computational & data science, and particularly big data, analytics and cybersecurity are key research areas at LSU that are spearheaded and facilitated by CCT. CCT is partnering with industry giants such as IBM, which serves as the perfect complement to LSU 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 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.

K.T. Valsaraj, PhD
LSU Vice President of Research & Economic Development

Message from the LSU CCT Director

I am extremely pleased to bring you the 2015-16 issue of Components that highlights the significant contributions of the LSU Center for Computation & Technology (CCT) to the university, the state and the nation. These contributions include a variety of ongoing multi-disciplinary research projects; leading the development of cyberinfrastructure in support of research; support of undergraduate and graduate education; 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.

I strongly believe that CCT provides a unique environment that promotes convergent research. We have continued to broaden our partnership with departments and colleges at LSU by hiring faculty members with a keen interest in multidisciplinary research. Three new tenure-track/tenured faculty members have come aboard since January 2015 (see page 47). Scott Hagen joins CCT and the Department of Civil & Environmental Engineering (CEE) as a tenured professor. Giulio Mariotti joins CCT and the Department of Oceanography & Coastal Sciences (DOCS) as a tenure-track assistant professor. Hagen and Mariotti have research interests in different aspects of coastal modeling. A third faculty member, Seungwon Yang, is a new tenure-track assistant professor jointly with the School of Library and Information Science. Seungwon's research interest is broadly in the area of data science. Currently, 36 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 15 departments in 8 different colleges (see page 6).

During the past year, CCT faculty members have continued to garner significant recognition for their work (see page 46). In April 2015, Jorge Pullin (CCT and Horace Hearne Chair in Theoretical Physics) was named an LSU Distinguished Research Master for 2014. Shawn W. Walker (Math and CCT) received the National Science Foundation CAREER award. Jesse Allison (Music and CCT) received the LSU Rainmakers Emerging Scholar Award. Also, Susanne C. Brenner was named the Nicholson Professor of Mathematics; the Nicholson Professorship of Mathematics is comparable to the Boyd Professorship at LSU.

At CCT, we have seen continued advancements in research and cyberinfrastructure and supporting LSU's educational and research mission. In the last year, CCT faculty and research staff members have received more than \$11 million in new grants, of which nearly \$10 million is from federal sources. They led or participated in proposals submissions with total requested funding exceeding \$90 million. We have expanded our



collaboration to several new areas, e.g., medical and biomedical informatics, social science research addressing aspects of coastal resiliency, quantum information science, cognitive psychology and learning, and studying interactions between drugs and their molecular targets at the systems level. The center, along with the Office of Research and Economic Development and the Louisiana Biomedical Research Network, acquired and installed a new IBM POWER8 based supercomputer named Delta. The unique design of Delta—housed at CCT—provides a new way of conducting computational research to LSU and the state (see page 36). CCT and LSU have developed a strong partnership with IBM. The deployment of Delta is part of a series of ongoing collaborations with IBM to facilitate big data research in the state.

On the education front, the Louisiana Board of Regents approved the Digital Media Arts & Engineering master's degree program, headed by Marc Aubanel, in collaboration with LSU's College of Engineering. The program is scheduled to graduate its first students in December 2016.

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

I hope that you will enjoy reading the articles about our research and other activities at CCT and will visit our website (<http://cct.lsu.edu>) for more details.

J. "Ram" Ramanujam, PhD
CCT Director

FACULTY BY FOCUS AREA



- ENGINEERING**
- Civil
 - Chemical
 - Petroleum
 - Electrical & Computer
 - Computer Science

- MUSIC & DRAMATIC ARTS**
- School of Music

- SCIENCE**
- Physics
 - Math
 - Biology
 - Chemistry

- BUSINESS**
- ISDS

- COLLEGE OF ART & DESIGN**

- SCHOOL OF MASS COMMUNICATION**

- COLLEGE OF THE COAST & ENVIROMENT**
- Oceanography & Coastal Sciences

- COLLEGE OF HUMAN SCIENCES & EDUCATION**

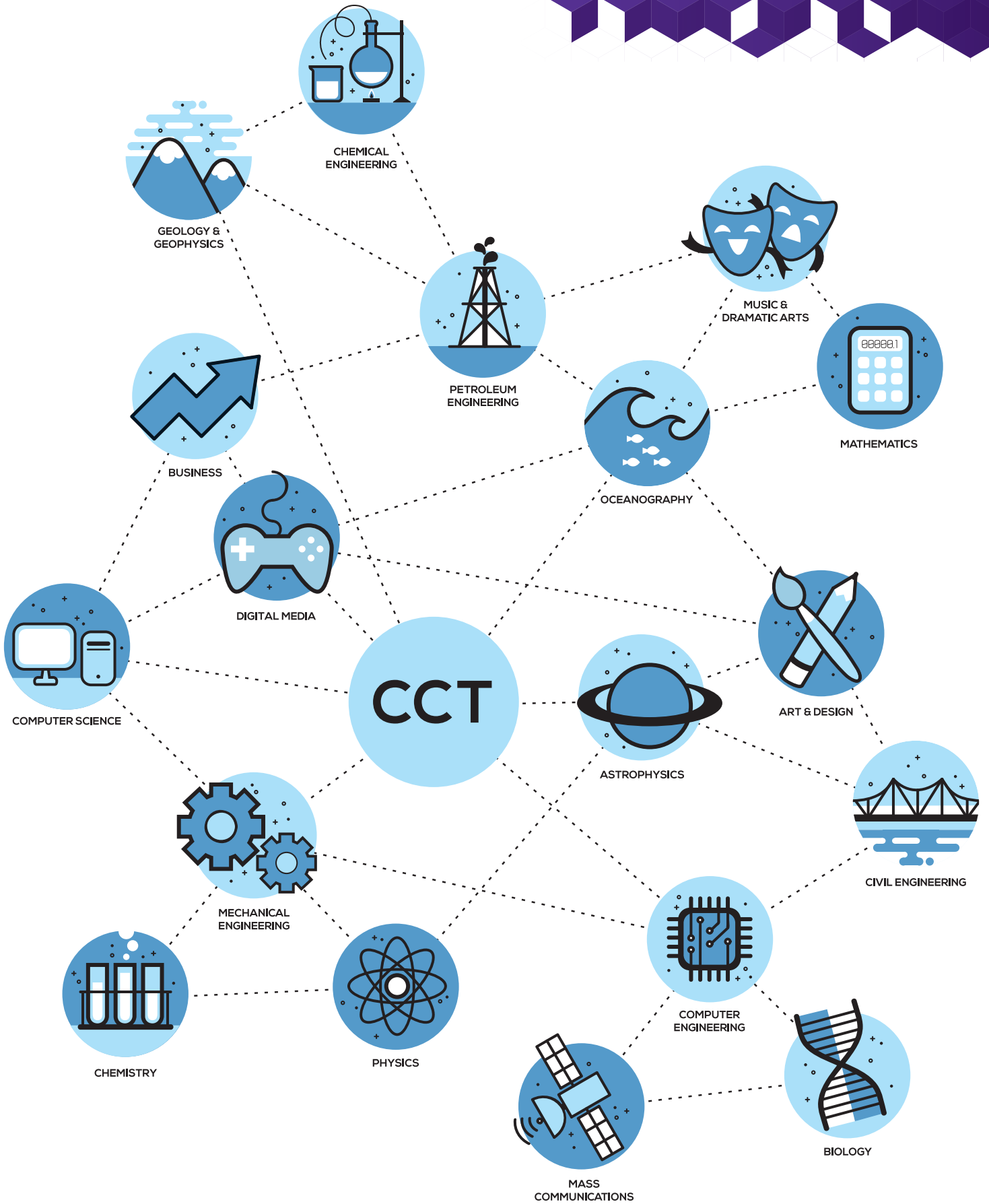
Core Computational Science focuses on the development of mathematical methods, software algorithms and the hardware to enable analysis of a broad array of complex problems on high performance computers and across high performance networks.

System Science and Engineering develops scalable programming models, compilation and runtime techniques, software libraries, 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, chemical engineering and systems biology, all of which rely heavily on molecular dynamics and related numerical techniques.

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

Cultural Computing explores complex computational and data driven applications in the humanities, arts and social & behavioral sciences, exploring the intersection of technology and creativity, and how computational and data technologies engage these disciplines. Examples include digital art and expression, technology adoption, and digital media.





Research Spotlight on the LSU Center for Coastal Resiliency

The LSU Center for Coastal Resiliency (CCR) is focused on the advancement and application of computational hydrodynamic and hydrologic models to include overland flow, river discharge, tides, wind-waves and hurricane storm surge. **Scott Hagen**, joint faculty at the Center for Computation & Technology (CCT) with the Department of Civil and Environmental Engineering is the CCR's director.

CCR is developing advanced systems-based models for the assessment of the effects of climate change and associated sea level rise, oil transport and fate, the Gulf dead zone and rainfall-induced flooding. Direct benefits include a better understanding of the dynamic, interrelated processes of natural and human systems and the ability to analyze impacts to the overall system at the coastal land margin.

Extensive interdisciplinary research experience enables the LSU CCR to effectively collaborate with natural and social scientists, engineers, government agencies, and stakeholders. The CCR is authorized by the Louisiana Board of Regents.

See more at www.lsu.edu/ccr.

Coastal Dynamics of Sea Level Rise

Coastal systems are dynamic. By definition, this means that they are characterized by perpetual change. Since the system itself is dynamic, it follows that most of its processes are dynamic as well. This is especially true for coastal waters with their ever-changing tides, waves and currents. Furthermore, long-term processes such as sea level rise change the coastal landscape by reshaping beaches, inundating marshes and exploiting infrastructure, all of which fundamentally change the physics of the system.

A New Paradigm in Coastal Modeling

With support from the National Oceanic and Atmospheric Administration (NOAA) National Centers for Coastal Ocean

Science, CCR faculty and students and their research partners at LSU, University of South Carolina, Florida State University and the University of Central Florida have built sophisticated computer models that incorporate state-of-the-art descriptions of the sea floor, coastal floodplains, land use and historic weather conditions. After verifying results from these models against historically measured water levels, the real fun begins. They then use their models to simulate changes to the environment such as shoreline position, vegetation density, population growth and sea level rise.

In a paper published in the American Geophysical Union's Geophysical Research Letters, CCR research scientist **Matthew Bilskie** (along with Hagen) explored the effects of sea level rise on the Mississippi coast. Using Hurricane Katrina from 2005 as a backdrop, the authors simulated what could have happened if it had struck in the year 2050 when sea level was 6, 12 or 18 inches higher than it was in 2005. In addition, they also went back in time to 1960 when the sea level was about 5 inches lower. Their findings indicate that coastal systems are sensitive to all of these factors and that these changes should be considered for all sea level rise assessments.

This work is being continued over the next several years with particular focus on ecosystems service valuation for the incorporation of natural and nature-based features to mitigate nuisance flooding and storm surge under present and future conditions.

Hagen and his team are also developing high-resolution tidal inundation and marsh productivity models for several estuaries along the mid-Atlantic and northeast U.S. coast for the U.S. Fish & Wildlife Service. The modeling platform, named Hydro-MEM, captures the interrelated hydrodynamic and biological processes and is able to simulate salt marsh productivity under present conditions in addition to a variety of climate change and sea level

Opposite page: Topography and bathymetry for the high-resolution ADCIRC model for the northern Gulf of Mexico region. The model contains 5.5 million computational points. The model takes 12 hours on 520 computational cores to simulate waves, water levels and depth-averaged currents for a single hurricane event.



Scott Hagen

rise scenarios. Similar to coastal Louisiana, portions of Hampton Roads, VA, are undergoing substantial rates of subsidence.

Knowledge gained in the northern Gulf of Mexico is being applied through an additional NOAA grant to develop models and tools to assess the effects of climate change on nuisance and storm surge flooding in the Hampton Roads region.

Better Views of the Gulf

The Department of Homeland Security is funding another research project, “Development of an Optimized Hurricane Storm Surge–Wave Model for the Northern Gulf of Mexico for use with the ADCIRC Surge Guidance System.” CCR, in collaboration with UCF, aims to improve the efficiency of ADCIRC Surge Guidance System (ASGS) through model enhancements as well as expanding the coverage of the ASGS to incorporate the coastal flood plains of Mississippi, Alabama and the Florida panhandle.

ADCIRC is a system of computer programs for solving time-dependent, free-surface circulation and transport problems in two and three dimensions. These programs utilize the finite element method in space allowing the use of highly flexible, unstructured grids. ADCIRC runs on a static mesh system, which digitally recreates natural geographical features. While a research-oriented mesh provides an effective representation of the coastal floodplain, it requires extensive supercomputing power.

Hagen’s team works to redefine the research-grade meshes for the northern Gulf of Mexico to enable real-time forecasting capability. The redefinition is done through several methods, such as identifying active floodplains and removing unnecessary elements from the computation. They also plan to improve the model’s efficiency by reducing the number of computational points for high-elevation natural features and enforcing stricter criteria for including vertical features (which take more time to

generate) in the model.

This project includes testing novel terrain analysis techniques, such as using a LIDAR-based system to determine the “roughness” of a particular surface (how often the terrain changes) at the regional scale. This method will significantly reduce the calculation time, down to 1-2 hours from an original time frame of roughly 12 hours. This allows for reasonable real-time forecasts as soon as meteorological predictions are made.

Benefits to Louisiana

CCR is a major contributor to LSU’s National Science Foundation Coastal SEES grant, led by Robert Twilley. Doctoral student **Chris Siverd** is building on the years of experience to develop historical tide and surge models for coastal Louisiana that span from 1850 to the present day.

A Louisiana Sea Grant College program grant is enabling a CCT team to update topographic elevations to the CPRA Coastal Master Plan model and enhance it for real-time forecasts that are visualized through the Coastal Emergency Risks Assessment tool (<http://cera.cct.lsu.edu/>).

A recent NSF RAPID response grant will examine the basis for incorporating rainfall-induced flooding into the Louisiana coastal surge model. Together with many collaborators from near and far, CCR produces transdisciplinary research and provides effective tools and products that enhance coastal resiliency.

The Cactus Computational Framework and the Einstein Toolkit



By Steven R. Brandt

Cactus is an open source problem solving environment designed for scientists and engineers. Its modular structure easily enables parallel computation across different architectures and collaborative code development between different groups from all over the world. Cactus originated in the academic research community, where it was developed and used over many years by a large international collaboration of physicists and computational scientists.

The Einstein Toolkit is a suite of codes used to 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 researchers **Steven R. Brandt**, **Peter Diener** and **Frank Löffler**.

Loop Quantum Cosmology

The observational discovery of the expansion of the universe in the 1920s is the foundation of modern cosmology. Among current cosmology theories, the Big Bang theory is in very good agreement with highly accurate observations of large scale galaxy structures and the cosmic microwave background radiation (CMB). In the Big Bang theory, the universe started

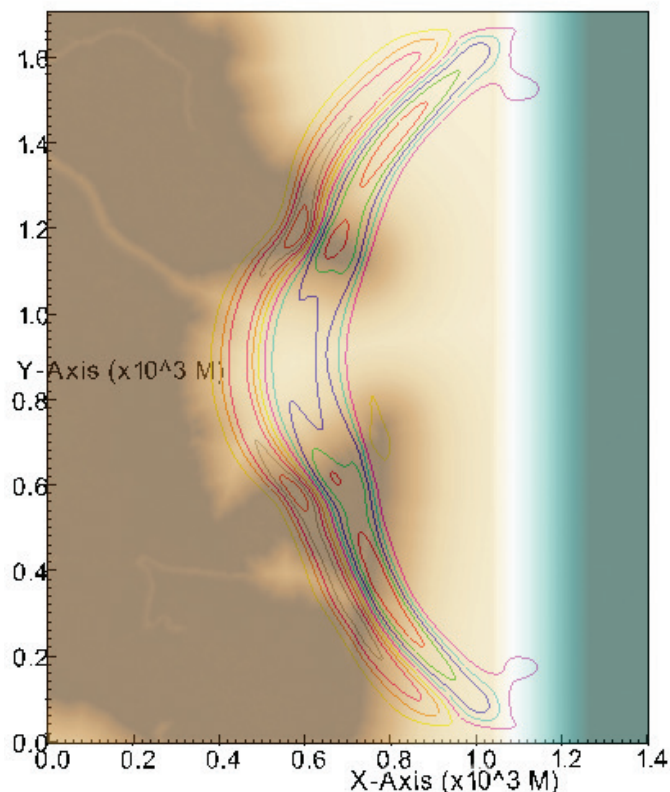
expanding from an infinitely hot and infinitely dense phase (the Big Bang singularity) and due to the expansion later cooled down enough that matter could form neutral atoms that could collapse gravitationally and form galaxies, stars, planets and everything else we see in the universe.

However, this classical picture does not take into account that quantum effects (as well as gravity) are important near the Big Bang singularity. We do not yet have a complete theory of quantum gravity, but Loop Quantum Gravity (LQG) is a promising candidate. When LQG techniques are applied to simple classical cosmological space-times (Loop Quantum Cosmology), it is found that quantum effects are very important and the Big Bang singularity is replaced by a Big Bounce, where a contracting universe (through quantum gravity effects) bounces and becomes our expanding universe.

The team has developed a Cactus-based code for performing large scale simulations of this quantum bounce in more complicated cosmology space-times in order to test the robustness of the bounce and to find observational signatures of the bounce (e.g. in the CMB). The code runs at high efficiency and can utilize CPUs, GPUs and Intel Xeon Phi.

Neutron Stars

The toolkit is also used to study the merger and instabilities of neutron stars. Neutron star instabilities teach us about the laws of physics and the behavior of very dense matter (i.e. where one teaspoon of neutron star material weighs millions of tons).



Opposite page: Three-dimensional visualization of the disk-like remnant from a binary neutron star merger just after black hole formation. This disk is relatively low-density (compared to the interior of the neutron star) and will eventually also fall into the black hole, but for some amount of time the remaining angular momentum prevents prompt collapse.

Left: Overlay of a wave contour striking the coast.

Recent results obtained by a collaboration between CCT and Parma University in Italy show how, using only publically available codes, anyone can model a merger of two neutron stars in full general relativity, using nothing more than a laptop for a good qualitative result in agreement with other published work. This work is the foundation upon which further studies of observed systems will be built, with the aim of uncovering the nature of the interior of neutron stars by observing their mergers.

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 for good, quantitatively correct results, and they remain challenging, however, even when using these powerful machines.

Chemora

For the past two years 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.

Chemora takes stencil codes written in a high level language and translates them to highly tuned GPU code by means of a performance model, using parameters obtained from micro-benchmarks. Because Chemora can choose tile size and memory strategies by consulting its model instead of compiling and running test codes, it can search a much larger optimization space than other similar stencil frameworks.

Coastal Simulations

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.

CaFunwave is a Cactus-based C++ implementation of the Funwave TVD code developed at the University of Delaware by **Fengyan Shi**. The Cactus implementation has been modified to include immersive boundaries, vegetation and to make some use of fixed mesh refinement.

Learn more at <http://cactuscode.org> and <http://einsteintoolkit.org>.

Stepping into Computing's Future with Release of HPX v1.0



STE||AR Group contributors (1) USA, (2) Argentina, (3) Spain, (4) France, (5) Switzerland, (6) Italy, (7) Germany, (8) Poland, (9) Sweden, (10) Russia, (11) China and (12) India

The **Systems, Technology, Emergent Parallelism & Algorithm Research (STE||AR, pronounced stellar)** Group is proud to announce the release of High Performance ParalleX (HPX) v1.0 with the feature complete release of a parallel runtime system that builds upon C++ computer language standards to facilitate distributed operations, enable fine-grained constraint based parallelism and support runtime adaptive resource management. Essentially HPX is moving from its beta phase to a fully functional system that takes the next step in the future of computing.

HPX is used by scientists and developers in a broad range of scientific applications to write code that scales better and performs more efficiently than conventional programming models.

"HPX version 1.0 is a major milestone for the STE||AR Group," said **Hartmut Kaiser**, group lead and senior researcher at CCT. "We're improving the utilization of computing and its resources, and HPX is the vehicle with which we are undertaking that."

The STE||AR Group's identity goes beyond national borders and includes faculty, researchers and students from 12 countries around the globe that find new and more efficient ways to utilize computers.

STE||AR is integrated into other areas of research at the Center as well as across the LSU campus. At

Simulation of a white dwarf star

LSU, nine post docs and graduate students are a part of the group and have the opportunity to work using cutting-edge technology.

The group's work on HPX is based on the widely used, international standard language C++. "HPX is driving the next international standards, and we're establishing HPX as something universally accepted," Kaiser said.

The HPX library enables application developers to write massively parallel, highly scalable codes using a modern multi-paradigm API. HPX portably supports heterogeneous runs on conventional and future architectures such as x86, Blue Gene, Xeon Phi, ARM and Epiphany.

Currently there are four grants from National Science Foundation and Department of Energy supporting HPX: XPRESS, STORM, PXFS and STAR.

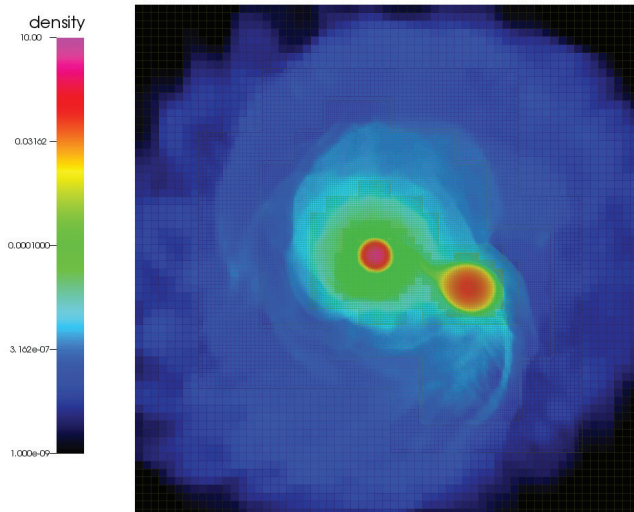
XPRESS, eXascale Programming Environment and System Software, is a project which funds the basic research into the underlying design and architecture of HPX; HPX v1.0 will be the final deliverable for the XPRESS project.

A Scalable Toolkit for an Open community supporting near Realtime high resolution coastal Modeling (STORM) is a project utilizing HPX to provide faster and more comprehensive tropical storm and hurricane forecasts. (See page 18 for more.)

PXFS, ParalleX File System, aims to extend the ParalleX execution model with a new input/output system to produce a new, highly innovative parallel execution model to allow researchers to develop highly efficient data management, discovery and analysis codes for big data applications covering a wide range of fields. (See page 14 for more.)

Scalable toolkit for Transformative Astrophysics Research (STAR) is a project using HPX to explore new techniques in the management of parallel execution and resource management to overcome the massive workload and communication requirements imposed by modern astrophysics simulations.

Geoffrey C. Clayton, professor in the LSU Department of Physics and Astronomy, explained that STAR uses HPX to write code to understand how binary white dwarf stars orbit each other with the possibility of merging. Due to the challenging aspects of the algorithms used in the simulation, the astrophysicists require a framework that would allow them to write code that could efficiently use the supercomputers at their disposal. HPX was deemed the perfect fit.



"STAR has been like a test bed for HPX," Clayton said. "It's been really great for moving HPX and STAR forward together on parallel tracks. We're simultaneously developing code to be used for science and showing the usability of HPX."

Learn more at <http://stellar.cct.lsu.edu> and <http://stellar-group.org>.

Improving Scientific Computing with ParalleX File System

High-performance computing involves increasingly larger amounts of data, and a three-university collaboration led by Clemson University with Indiana University and LSU is working to address these challenges.

PXFS, or **ParalleX File System**, uses the STE||AR Group's High Performance ParalleX (HPX) system, an implementation of ParalleX based on C++, and Clemson's OrangeFS, a high-performance parallel file system, to build a more robust toolchain that is changing the way scientific computing work is done.

The principal investigators for the PXFS grant from the National Science Foundation are **Walter B. Ligon III**, Parallel Architecture Research Laboratory, **Clemson**; **Maciej Brodowicz**, Center for Research in Extreme Scale Technologies at Indiana; and **Hartmut Kaiser**, senior researcher at Center for Computation & Technology (CCT) at LSU and head of the STE||AR group. Based in LSU's CCT, the **Systems Technology, Emergent Parallelism & Algorithm Research** (STE||AR, pronounced stellar) Group includes faculty, researchers and students from around the world who find new and more efficient ways to use computers. (See page 12 for more about STE||AR and HPX.)

The PXFS team's goal is to extend the ParalleX execution model to include a new model of input/output (I/O) to allow researchers to develop highly efficient data management, discovery and analysis codes for big data applications. The team realized their initial approach would require end-users to have a thorough knowledge of HPX to use the file system, which isn't always realistic.

To help solve this challenge **Chris Branton**, then IT consultant at CCT and adjunct professor in LSU's Department of Computer Science & Engineering (as of August 2016, assistant professor of computer science at Drury University in Springfield, MO), was brought into the project to further develop workflows and eventually an application programming interface (API) to improve the usability of PXFS.

This project will help end users take advantage of the new features provided by HPX and OrangeFS in an intuitive way.

Branton's work on PXFS is focused on improving human-computer interaction for the research of **Alex Feltus**, associate professor in the Genetics and Biochemistry Department at Clemson.

Feltus works in agricultural genetics identifying genes that control agronomic traits to improve crop yield and produce larger biomass crops. His research generates a huge amount of data that must be processed on a supercomputer and is the first project to use PXFS.



Chris Branton

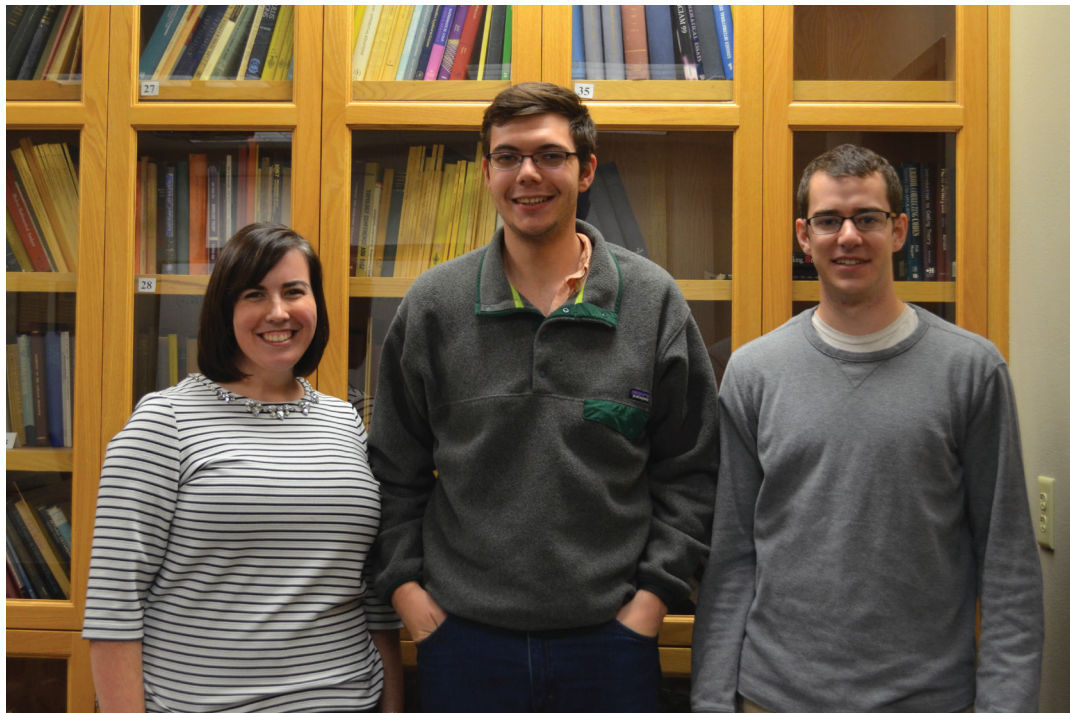
"I'm reaching a massive bottleneck of taking weeks to process the data," Feltus said. "I need to be able to process it faster - the sooner I can process the sooner I can determine if what I found on the computer is real in real life."

PXFS is meant to help orchestrate storage and processing of these massive, highly variable data sets to improve overall throughput of the data in existing workflows.

"We're working to understand where greater performance can be had," Branton said. "We're working to develop a set of tools for Alex's work to help figure out what the PXFS API will need to do."

This work will bring HPX more firmly into the big data arena and can be applied beyond biology as well, Branton said.

Preparing Undergraduates for Success with a Computational Math Concentration



Jessica Wojtkiewicz, George Owen and Daniel Bourgeois

Credit: Susanne C. Brenner

The second group of students completing their degrees with a concentration in computational math from Louisiana State University includes **Jessica Wojtkiewicz**, **George Owen** and **Daniel Bourgeois**.

Students who earn a degree with the concentration are required to complete four courses: numerical linear algebra, numerical differential equations, numerical analysis and optimization. Students are also encouraged to complete a summer research experience before graduation with a Research for Undergraduates (REU) program and/or an internship.

“These research experiences and internships provide real-world experience making for more successful careers, whether our students pursue graduate school or begin working in industry after graduation,” said **Susanne C. Brenner**, Nicholson Professor of Mathematics at LSU and Core Computational Science focus area lead at the Center for Computation & Technology (CCT).

Wojtkiewicz participated in the University of Maryland, Baltimore County (UMBC) High Performance Computing REU program in summer 2015 where she was part of a group that worked with a mathematical model of pancreatic beta cells provided by the National Institutes of Health. These cells are responsible for insulin secretion. Wojtkiewicz presented her research results at the International Symposium on Biomathematics and Ecology Education and Research at Illinois

State University, Scientific Computing Around Louisiana workshop (see page 32) and at an LSU College of Science dinner honoring their donors. Wojtkiewicz graduated in December 2015 and plans to attend graduate school.

Bourgeois completed an internship at Sandia National Laboratories in summer 2016, and Owen participated in the 2016 UMBC REU program. Bourgeois and Owen will graduate during the next academic year.

The first students to graduate with this concentration were **Rachael Keller**, **Bruno Beltran** and **Benjamin Birk**, and they received their degrees in spring 2015. Keller and Beltran received National Science Foundation Graduate Research Fellowships. Keller is a graduate student in applied mathematics at Columbia University. Beltran is a graduate student in the Chemical and Systems Biology Program at Stanford University. Birk is employed by Microsoft, where he worked as a student during his summer research experiences as an LSU undergraduate.

The Core Computational Science focus area faculty at CCT who have joint appointments with the LSU Department of Mathematics created this concentration.

Students interested in the computational math concentration should contact Brenner.

Coastal Resilience Collaboratory

Modern river deltas are disappearing due to global reductions in river sediment, land subsidence and rising sea level, causing significant threats to natural and human systems. Hundreds of billions of dollars may be needed to secure human communities in sensitive coastal environments. Driven by a complex web of data collection, analysis, and computer simulation to sustain deltaic coasts, this requires a systematic approach for integrating the vast quantities of collected and numerical simulations data.

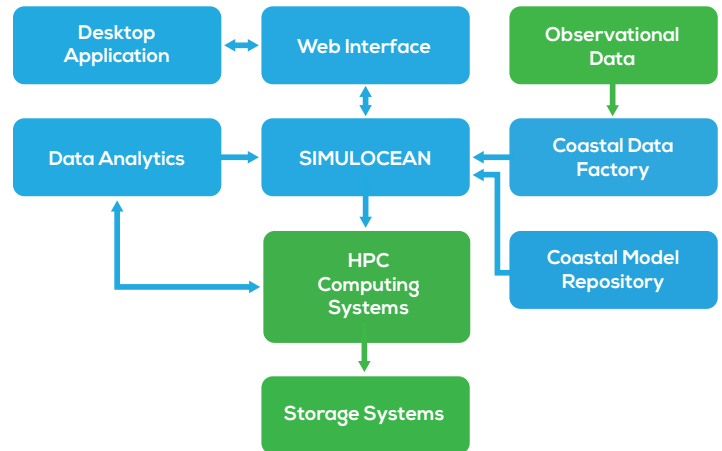
The Coastal Resilience Collaboratory (CRC), funded by the National Science Foundation (NSF) Cyber SEES program, is building an integrated, coupled modeling framework on top of a platform-transparent cloud technology tailored for the coastal modeling community. The primary focus is to facilitate the deployment of complex models on cloud and cloud-like architectures with negligible performance overhead through use of low-level virtualization technology. The CRC uses two large river deltaic systems, the Mississippi River Delta in the United States and the Mekong River Delta in Vietnam, to serve as models for the application framework and to address coastal sustainability issues.

Interdisciplinary Collaboration

The CRC project is one of the outcomes of the Northern Gulf Coastal Hazards Collaboratory (NG-CHC) previously funded by the NSF EPSCoR program. The CRC, led by **Q. Jim Chen**, CSRS Distinguished Professor in Coastal Engineering and Professor of Civil and Environmental Engineering at LSU and Coast to Cosmos focus area lead at the Center for Computation & Technology (CCT), has been interacting with currently funded NSF/CNH (NSF Coupled Natural-Human Dynamics) and NSF Coastal SEES projects by demonstrating the utility of simulation management systems and cloud computing to support modeling frameworks, including population change modeling and simulation validated through empirical surveys. The CRC research team consists of researchers in Civil and Environmental Engineering, Oceanography and Coastal Sciences, Environmental Science, Computer Science and Engineering, Geology and Geophysics, and CCT.

Cloud-ready Cyberinfrastructure

Compared to the quick adoption of cloud computing technology in industry, the academic community, especially the computational science community as a whole, has been slow to make the move, partly because of the lack of investment in cloud-ready systems from NSF and other major funding agencies. For years, many researchers and engineers who didn't run large-scale applications regularly were inhibited by the effort needed to gain the specialized knowledge needed to effectively use HPC resources for their research. Their time could be better spent on their research if they did not have to worry about how to run their applications. It was not a surprise that with the NSF Cloud initiative, NSF recently announced two \$10 million projects "Chameleon" and "CloudLab" to enable the academic research community to drive research on a new generation of innovative applications for cloud computing and cloud computing



SIMULOCEAN Science Gateway

architectures.

The Coastal Model Repository (CMR) is targeting such cloud and cloud-like architectures to enable quick deployment of coastal models and their working environments. CMR will serve as a community repository for precompiled open source models that are widely used by coastal researchers. While source code for various executables and libraries will be available, CMR will also introduce distribution of containerized coastal models, which can run on any cloud-like architecture directly, and with negligible system overhead.

The idea of containerization of cloud-ready applications is not new, but it has become a viable solution given the rapid development of kernel-level virtualization technologies. One such technology, Docker, is an open platform allowing developers to build, ship and run distributed applications in self-contained environments. Docker enables executable applications to be quickly assembled from components then run by a user without the need to rebuild or satisfy any external dependencies. As a result, a Docker-enabled application can be reliably executed in a known operating system environment on any system that supports Docker containers.

With the help of CMR, a coastal researcher can start running state-of-the-art models on the latest cloud-ready computing systems in minutes. Workflow management tools, such as SIMULOCEAN, can take advantage of CMR to quickly deploy coastal models on academic and commercial cloud platforms while continuing their support on traditional HPC systems.

Docker supports applications that make use of accelerators (GPUs). One of the critical codes to be enabled by our cloud framework is CaFunwave, an implementation of Funwave-TVD in C++ using the Cactus framework (see page 10). CaFunwave will make use of the Chemora accelerator framework for Cactus (<http://einstein toolkit.org>) to make better use of modern HPC

resources, such as SuperMIC and QueenBee2 at LSU.

Simulocean (<http://simulocean.org>) is a web-based deployment and visualization framework for coastal modeling and beyond. As shown in the diagram here, Simulocean collects observational data, schedules modeling codes for execution, manages data transfer, and visualizes both observational and numerical results. With all the information collected, Simulocean can also provide direct validation and verification for models, and generate high quality technical reports. Simulocean serves as the frontend

of four processing subsystems of the CRC cyberinfrastructure: (1) observation data assembling, (2) model distribution and deployment, (3) workflow management, and (4) numerical data interpretation and visualization.

The CRC team is currently collaborating with research staff via the Extended Collaborative Support Service (ECSS) at XSEDE to make Simulocean a science gateway for the XSEDE resources.

See <http://crc.cct.lsu.edu> for more.

Viewing Communication and Computation through a Quantum Lens

Mark M. Wilde, assistant professor in physics and astronomy with a joint appointment with the Center for Computation & Technology, pursues research in an area known as quantum information science. The main questions driving his research are: What are the ultimate limits that nature imposes on communication and computation, and what are effective procedures for achieving these limits?

In order to answer these questions convincingly, one must reassess the theories of information and computation under a “quantum lens.” That is, since quantum mechanics represents our best understanding of microscopic physical phenomena and since information is ultimately encoded into a physical system of some form, it is necessary to revise the laws of information and computation established many years ago by intellectual giants such as Shannon and Turing.

This is not merely an academic exercise but instead represents one of the most exciting new frontiers for physics, mathematics, computer science and engineering. Entanglement, superposition and interference are all aspects of quantum theory that were once regarded as strange and in some cases, nuisances. However, nowadays, researchers understand these phenomena to be features that are the enabling fuel for a new quantum theory of information and computation, in which seemingly magical possibilities such as teleportation are becoming reality.

Several notable examples are computational speedups in quantum computing, increased communication capacities of noisy communication channels, secure encryption based on physical principles (called quantum key distribution) and enhanced precision in measurements. Concepts developed in the context of quantum information theory are now influencing other areas of physics as well, such as quantum gravity, condensed matter and thermodynamics.

A recent research success of Wilde’s is the development of a bound on the amount of secret key that can be generated in a quantum key distribution protocol, if the participants in the



Mark M. Wilde

protocol do not have access to a quantum repeater device. This bound is now being used as a benchmark by U.S. government agencies to determine whether experimentalists have implemented a quantum repeater device (a quantum repeater is essential for extending the distance over which a secret key can be generated).

Wilde is also the first to develop a rigorous framework for quantifying secret key communication capacities in which realistic energy constraints are taken into account.

In May 2015, Wilde proved a physically meaningful enhancement of a 40-year-old theorem known as the *quantum data processing inequality*, which underlies nearly all the communication bounds of quantum information theory. He has now applied this theorem in a variety of contexts, to sharpen the uncertainty principle of quantum mechanics, the second law of thermodynamics and the no-cloning theorem of quantum information.



Zachary Byerly discusses code implementation details with Hartmut Kaiser.

Credit: LSU University Relations

STORM Project Working to Improve Storm Surge Prediction and Coastal Safety

Tropical storm and hurricane forecasting is being improved thanks to work being done by researchers at LSU's Center for Computation & Technology (CCT), Notre Dame, University of North Carolina and the University of Texas at Austin.

STORM, a Scalable Toolkit for an Open community supporting near Realtime high resolution coastal Modeling, is a four-year, National Science Foundation-funded collaborative project among the four universities.

"STORM will allow us the capability to improve the performance of the ADCIRC tool and will help us improve the safety of populations living along the coasts," said **Hartmut Kaiser**, CCT researcher, a STORM principal investigator and lead of the Systems Technology, Emergent Parallelism & Algorithm Research (STE||AR, pronounced stellar) group housed at CCT.

Along with CCT's Kaiser, **Joannes Westerink** of Notre Dame, **Rick Leutich** of UNC and **Clint Dawson** of UT Austin are principal investigators on the NSF grant.

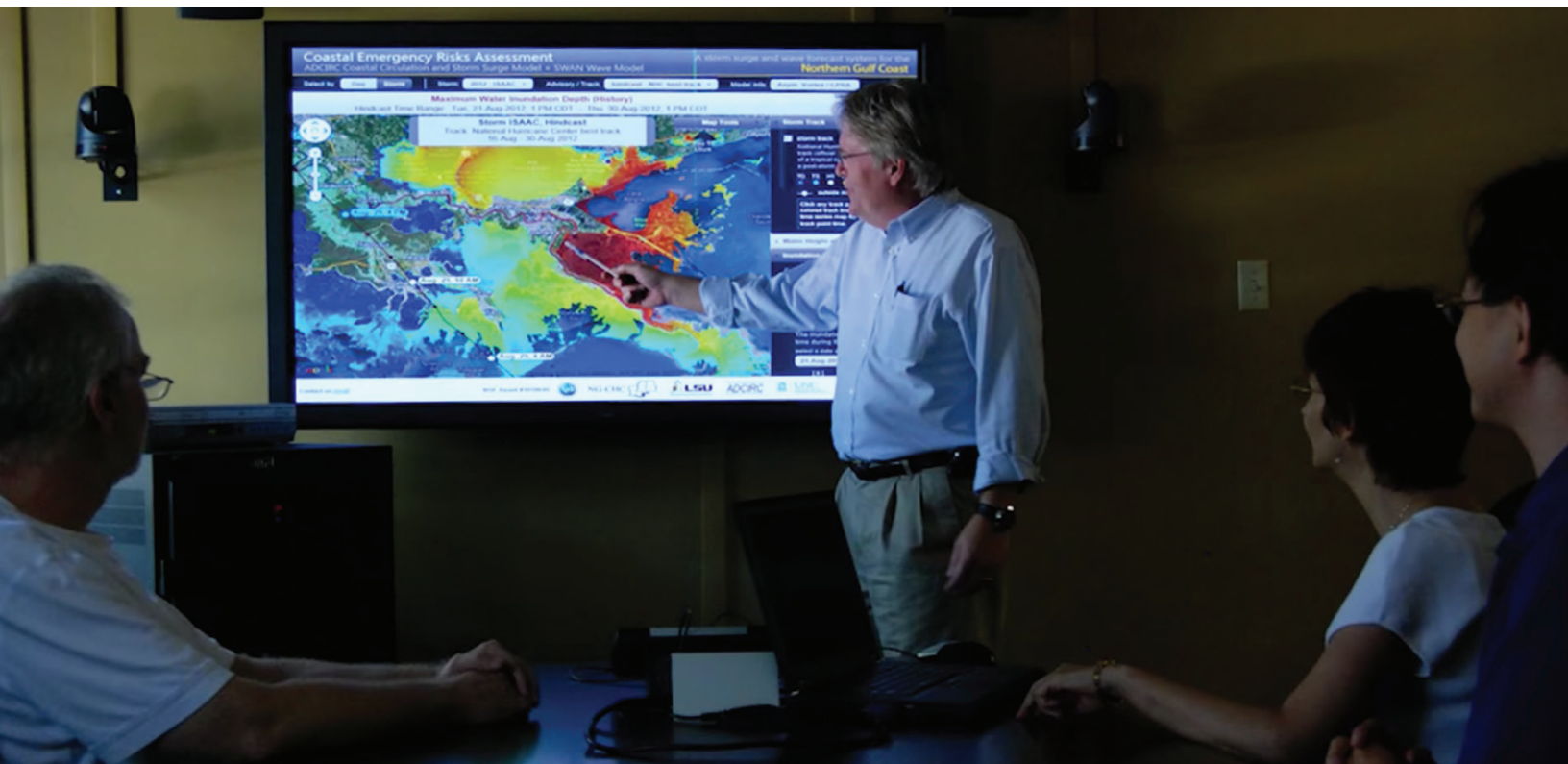
ADCIRC, Advanced Circulation and Storm Surge model, is a

critical community resource used around the globe to predict areas that will flood during tropical storms and hurricanes. 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.

STORM brings together researchers from computer science, coastal science and engineering to broaden ADCIRC from a successful but somewhat static model into a dynamic, multi-algorithmic modeling environment.

"We're updating ADCIRC so that it runs more efficiently on today's larger supercomputers, while still delivering the same accurate results that emergency managers need in a timely fashion in the event of a hurricane," said **Zachary Byerly**, postdoctoral researcher at LSU CCT working on STORM.

STORM incorporates High Performance ParalleX (HPX) into ADCIRC to parallelize code and run it on supercomputers. HPX is the first open source implementation of the ParalleX execution



Robert Twilley, co-PI and director of Louisiana Sea Grant, uses the Coastal Emergency Risks Assessment (CERA) visualization tool, developed at LSU by Carola Kaiser, to show results of an ADCIRC simulation of Hurricane Isaac.

model and modern runtime system developed by the STE||AR group (see page 12 for more).

Now at the end of its second year, STORM has built on the success of its first year and reached another major milestone: running a full tropical cyclone simulation on multiple compute nodes with the discontinuous Galerkin version of the ADCIRC code, DGSWEM, using the libraries LibGeoDecomp and HPX for parallelization. The team was able to reach this important goal thanks to progress on both the computer science libraries and the Fortran physics modules.

In June 2016, Byerly traveled to Germany for two weeks to collaborate closely with **Andreas Schäfer** (Friedrich-Alexander University Erlangen-Nürnberg), the creator and chief developer of LibGeoDecomp, an auto-parallelizing library for computer simulations of any scale. Together they wrote a new HPX parallelization back-end for LibGeoDecomp that utilizes the dataflow function of HPX and allows the code to run efficiently on a large number of compute nodes.

“This is a tremendous leap forward for the code, as it enables static load balancing and paves the way for dynamic load balancing,” Byerly said. “Load balancing is critical, especially for this problem – it allows us to put the computing power exactly where the simulation needs it.”

“We have also worked hard to implement, test and verify more

physics functionality in the Fortran part of the code,” Byerly said. “Having a code that runs fast is great, but for a real-world code, getting the right answer from the code is critical – we have to carefully test every new feature by running a variety of problems and comparing the results to a reference code.”

Steven Brus and **Max Bremer**, graduate students at Notre Dame and UT, respectively, have contributed a great deal.

“Right now the version of ADCIRC in production doesn’t really have load balancing, so parts of the computer essentially sit unused during the simulation, which is inefficient,” Byerly said. “When we can take the HPX version and get it running on multiple compute nodes we will be able to put all the computing power exactly where the simulation needs it.”

The STORM team presented several talks in January 2016 during the Second Symposium on High-Performance Computing (HPC) for Weather, Water and Climate at the American Meteorological Society’s 96th Annual Meeting in New Orleans. Results from STORM work are also making an impact internationally. Byerly presented a conference paper at the International Workshop on Legacy HPC Application Migration in Sapporo, Japan, in December 2015.

Learn more at <http://storm.stellar-group.org>.

Speeding Up Discovery of New Pharmaceuticals at CCT



Michal Brylinski

The administration of drugs is a key strategy in pharmacotherapy to treat diseases. Drugs are typically developed to modulate the function of specific proteins, which are directly associated with particular disease states. Recent studies suggest that protein-drug interactions are rather promiscuous, and the majority of pharmaceuticals exhibit activity against multiple, often unrelated proteins. Clearly, this binding promiscuity significantly complicates the development of new drugs.

Led by **Michal Brylinski**, assistant professor with joint appointment in the Department of Biological Sciences and the Center for Computation & Technology (CCT), the Computational Systems Biology Group at LSU has recently been awarded a nearly \$1 million research grant by the National Institute of General Medical Sciences.

The project will study interactions between drugs and their molecular targets at the systems level. This innovative research holds significant promise in advancing human health through the development of multi-target drugs for polypharmacology as well as the identification of novel targets and off-targets for existing drugs. Polypharmacology is the design or use of pharmaceutical agents that act on multiple targets or disease pathways.

eFindSite

“In collaboration with other research groups at LSU, we have already developed a number of new algorithms and high-performance codes for computer-aided drug discovery,” Brylinski said. “One of our first tools was eFindSite, a template-based modeling approach to accurately identify drug binding sites and binding residues across large datasets of protein targets. This research was stimulated by continuing advances in genome sequencing technologies that gave rise to the rapid accumulation of raw genomic data. An efficient annotation of this massive volume of biological sequences is currently one of the biggest challenges in biomedicine.”

Brylinski and his team developed eFindSite that combines state-of-the-art protein threading and structure alignment algorithms with machine learning. This allows researchers to make reliable predictions using only weakly homologous templates selected from the so-called “twilight zone” of sequence similarity. Currently, this is one of the most accurate algorithms to identify drug-binding sites within a given proteome. It was also the first code the team parallelized and ported to hardware accelerators with significant speedups.

When compared to the serial version, parallel eFindSite runs 17.6× times faster on a hybrid system composed of a multicore processor and an Intel Xeon Phi accelerator. This work is featured in the 2015 book, “High Performance Parallelism Pearls: Multicore and Many-core Programming Approaches,” edited by **James Reinders** and **James Jeffers**.

GeauxDock

Another code developed in collaboration with the Technologies for Extreme Scale Computing (TESC) team at CCT and supported by the Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA) is GeauxDock. This molecular docking program can be used to perform structure-based virtual screening, which simulates the association between small organic molecules and their pharmacologically relevant protein targets. GeauxDock is a unique docking approach that features a descriptor-based scoring function integrating evolutionary constraints with physics-based energy terms, a mixed-resolution molecular representation of protein-ligand complexes and an efficient Monte Carlo sampling protocol.

Highly optimized docking codes are important for the effectiveness of virtual screening methods because of the large number of drug candidates to be evaluated. Developed specifically for heterogeneous computing platforms, the current version of GeauxDock can be deployed on modern multicore processors as well as massively parallel accelerators such as the Intel Xeon Phi and NVIDIA Graphics Processing Unit (GPU). Using a Xeon Phi gives 1.9x performance improvement over a dual 10-core Xeon CPU, whereas the best GPU accelerator, NVIDIA GeForce GTX 980, achieves a speedup as high as 3.5x. GeauxDock can take full advantage of modern heterogeneous architectures to considerably accelerate structure-based virtual screening applications. GeauxDock was selected by the editors of the Journal of Computational Chemistry for the front cover because it is well suited for proteome-scale applications utilizing the increasingly growing protein sequence and structural data.

eMatchSite

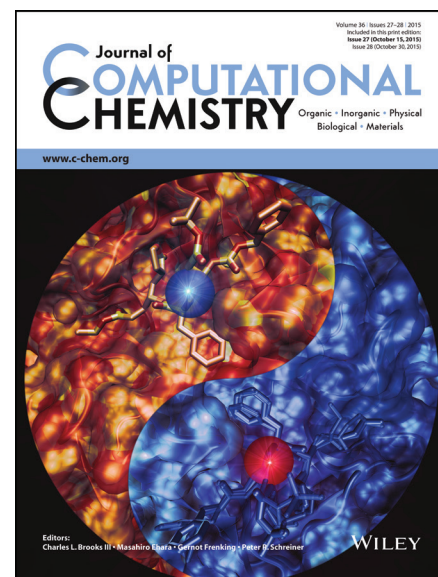
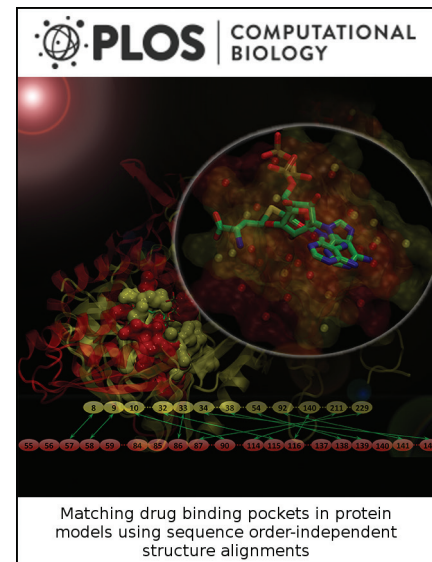
The inherent lack of selectivity of drugs often leads to drug side effects. On the other hand, these polypharmacological attributes can be used to develop a single drug that acts on multiple targets of a unique disease pathway, as well as to identify unknown targets for existing drugs, which is also known as drug repositioning.

At the outset of drug development and repurposing, computational approaches are typically used to detect those binding sites having the capability to bind similar compounds. Currently, methods employing sequence order-independent alignments are amongst the most accurate algorithms for drug binding site matching. However, many of these techniques require high-quality protein structures, which are unavailable for the majority of gene products.

To alleviate this issue, the Computational Systems Biology Group developed eMatchSite that constructs biologically correct drug binding site alignments using computer-generated protein models. eMatchSite calculates local binding site alignments using the Kuhn-Munkres algorithm with inter-residue distances estimated by machine learning. In addition, eMatchSite provides a calibrated significance score to identify those pockets capable of binding chemically similar ligands regardless of any global sequence and structure similarities among target proteins. Its unique feature is a high tolerance to structural distortions in drug binding regions. Constructing correct alignments using pockets predicted in protein models opens up the possibility to investigate protein-drug interaction networks for complete proteomes. Editors of PLoS Computational Biology selected eMatchSite for the front cover due to its remarkable potential for polypharmacology and rational drug repositioning.

In modern biological sciences, the key challenge has shifted from the study of single molecules to the exhaustive exploration of molecular interactions and biological processes at the level of complete proteomes. Understanding how complex living systems work can help find treatments for disorders of poorly understood etiology, such as cancer and neurodegenerative disorders. Systems biology requires truly multidisciplinary efforts at the intersection of biology, physics, chemistry and computer science.

"We are very fortunate to collaborate with so many talented researchers at LSU and to have strong institutional support and access to top-notch computing resources," Brylinski said. "We believe that our collaborative research will not only fundamentally advance our understanding of molecular networks but also utilize cutting-edge computer technology to support the development of novel therapies."



NSF Funds LSU Research Combining Social Science with Big Data Led by Nina Lam



Nina Lam



Michelle A. Meyer

The National Science Foundation (NSF) has funded a four-year Interdisciplinary Behavioral and Social Science (IBSS) Research Award to an LSU team that includes faculty in the Center for Computation & Technology (CCT).

Nina Lam, Abraham Distinguished Professor of Louisiana Environmental Studies in the Department of Environmental Sciences, is lead investigator of the more than \$800,000 project that will examine whether social and geographical disparities exist during the four phases of emergency management (mitigation, preparedness, response and recovery).

The team, which includes co-principal investigators **Michelle A. Meyer**, **Seung-Jong “Jay” Park**, **Margaret A. Reams**, **Seungwon Yang** and **Kisung Lee**, will do this by comparing Twitter data from two 2012 disaster events, Hurricane Isaac and Superstorm Sandy.

Park, professor in the Division of Computer Science and Engineering, and Yang, assistant professor in the School of Library and Information Sciences, both have joint appointments at CCT. Meyer is an assistant professor in the Department of Sociology, Reams is a professor in the Department of Environmental Sciences and Lee is an assistant professor in the Division of Computer Science and Engineering.

“Twitter data is very noisy,” Lam said. “And to make the data useful we need very good algorithms to process and clean the data to identify the content that is important.”

CCT’s computing power and analytics expertise will make that work possible and extract information useful for emergency management.

Ultimately the team will determine how big a problem of social and geographical disparities is in social media use and whether social media use may serve to overcome or further deepen disparities in each phase of emergency management.

“Our project is comprehensive and systematic and will advance both social science and information science research,” Lam said. “This is probably one of the first funded projects of social scientists working with CCT, and our team works well together blending social scientists with CCT and computer science & engineering.”

The knowledge gained from this project will help develop strategies to reduce disparities, create effective social media campaigns and emergency management outreach, and promote community resilience in the face of disasters.



Seung-Jong “Jay” Park



Margaret A. Reams



Seungwon Yang



Kisung Lee

Geometric and Visual Computing Group Develops Geometric Processing and Reconstruction Techniques

Cutting-edge 3D geometric modeling techniques being used by innovative researchers at the Center for Computation & Technology (CCT) are making a difference in a variety of fields.

Led by **Xin “Shane” Li**, Oskar R. Menton Professor in the School of Electrical Engineering & Computer Science and CCT, the Geometric and Visual Computing (GVC) Group conducts research on geometry and image data processing that has applications in forensics, medical research, archaeological tasks, and computer-aided design and manufacturing.

High-quality Regular Meshing for Scientific Computing

Li’s team has made great strides in its meshing model used for accurate simulation. In scientific simulations, curved geometries or regions are usually discretized using irregular meshes (e.g., triangular meshes for 2D space or surfaces, tetrahedral meshes for 3D space or solids). In contrast, discretization of general geometries using regular meshes (e.g., quadrilateral meshes for 2D space or surfaces, hexahedral meshes for 3D space or solids) could result in more efficient and accurate computing and more economic storage for many scientific computing tasks.

“We only need to use 10% to 25% the number of elements to obtain the same level of computation accuracy,” Li said. “The simulations on our regular tessellations indeed run faster and are more accurate than those on the conventional irregular tessellations.”

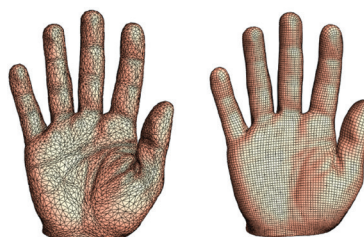
The GVC team is developing a new computational pipeline utilizing distributed high-performance computing (HPC) to process the regular meshing of large-scale geometric data in parallel and facilitate more efficient simulations in LSU’s HPC environments.

Digital Body Scanning and Modeling

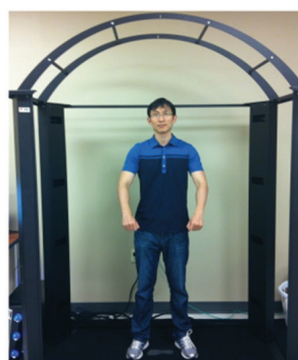
Working with researchers at the **Pennington Biomedical Research Center** in Baton Rouge, the GVC group is improving diabetes management with better physical profile information.

“Traditionally doctors use tape to get measurements of a person’s body,” Li said. “We have developed a digital modeling system using low-cost Microsoft Kinect sensors to obtain real-time 3D scan of human bodies and perform digital geometric measurement.”

A set of sensors is deployed to scan the body from multiple directions. Because the body cannot be fully covered in real-time scanning and there is inevitable self-occlusion, the partial scans need to be fused and the missing regions need to be completed. The GVC team developed novel geometric data stitching and completion techniques to reconstruct the 3D geometry. More than 100 subjects at Pennington.



High-quality regular mesh generation



Body scanning



Robotic environment reconstruction

Low-bandwidth Localization and Mapping for Autonomous Robots

The GVC group is also working on a robotics project. They have built a small robot, equipped with a RGB-D (for Red, Green, Blue plus Depth) sensor, to reconstruct and map a hazardous environment as it autonomously explores this environment.

Li explained that the two key challenges in this project are the highly dynamic and noisy sensing data obtained by the low-cost sensor and the limited bandwidth of data transmission.

“Due to its size and power-consumption limitations, the small robot could not carry high-resolution scanners and powerful workstations like a Google street view car,” Li said.

The GVC team has developed an environment reconstruction system using a navigating iRobot that carries an RGB-D sensor and a Raspberry Pi.

Making Strides in Experimental Music and Digital Art at CCT



Experimental Music + Digital Art Make Sweet Poetry through CCT

In March 2016 two faculty members at the Center for Computation & Technology (CCT) were part of an interactive poetry experience at Technology, Entertainment and Design at Louisiana State University (TEDxLSU). About 700 people attended *Diamonds in Dystopia*, an interactive, live-streaming poetry web app performance that took the audience through sensory decisions and the experience of creating a poem collectively.

Created by CCT's **Jesse Allison**, associate professor of Experimental Music & Digital Media; **Derick Ostrenko**, assistant professor of Digital Art; and poet **Vincent A. Cellucci**, the *Diamonds in Dystopia* performance used advanced coding

techniques to aggregate Ted Talk transcripts to generate a poem in real time.

Cellucci's poem *Bound by Digital Countries* was presented to the audience via their cell phones, and they could tap words and phrases that resonated with them to trigger Markov chain reactions, creatively data mining more than 2,500 TED talks to send stanzas and sounds to Cellucci on stage. The taps created a musical experience while contributing to the visual projection of the collectively created poem.

See the original poem and the TED-generated poem at <http://tedxlsu.emdm.io>

"It's an overwhelming experience but thematically appropriate," Allison said. "It moves your attention around - reading, listening and simply soaking it all in."

These types of performances are made possible with CCT's High-performance Interactive Visualization and Electroacoustics (HIVE) supercomputer, which began as a project during a Research for Undergraduates Experience (REU, see page 30) project.

HIVE was developed by researchers in LSU's Experimental Music & Digital Media (EMDM) and Digital Media Arts & Engineering programs repurposing retiring supercomputers Queen Bee and Phillip to create a cloud computer for art and music with real-time computing. Hundreds of people are able to work together at the same time using HIVE, a 448-core cloud-based platform built at CCT.



Feeling good vibrations: The FireFader8x allows a performer to control sound and feel virtual musical instruments at the same time. Each of the eight faders is connected to a motor (not shown), which can precisely push back on the faders according to a virtual physics simulation.

Touching Sound with Transmogrified Strings

Edgar Berdahl, an assistant professor in experimental music and digital media with a joint appointment at the Center for Computation & Technology (CCT), has created Transmogrified Strings, the first music composition performed using an easily portable, many degree-of-freedom haptic force-feedback control interface. This has been performed at CCT's Cinema for the Ears, the International Computer Music conference in Athens, Greece, the Society for Electro-Acoustic Music Conference in Blacksburg, VA, and the International Conference on New Interfaces for Musical Expression (NIME) in Baton Rouge (see page 26).

Berdahl's composition surprises the listener with sounds that are both new yet uncannily familiar. Virtual plucked strings can be tuned as low as 0.5Hz or as high as the upper bounds of human hearing. The virtual strings retain their tangible character even as the sound changes drastically, and the feel of the instruments changes too, which in turn affects the performer's interaction with the virtual strings.

Evaluating How Accurately Humans Can Operate Sensors

In the field of new instruments for musical expression, so many sensing technologies are available that it can be hard for instrument designers and human-computer interface designers to know which ones to choose.

CCT's Berdahl and **Michael Blandino**, assistant dean of the LSU Honors College, have invented a new information-theoretic approach for evaluating human-computer interaction using these sensors. According to the Shannon-Hartley theorem, the maximum number of bits of information that humans can communicate using these sensors can be estimated by having humans perform "Gaussian-distributed gestures."

Working with **Daniel Shanahan** and **David Baker** from the Music Cognition and Computation Lab at LSU, the team is assessing

a wide range of continuous sensors and further investigating how other theorems from telecommunications and information theory can be applied to study human control of sensors.

Simulating Virtual Physics 44,100 Times A Second

For virtual reality simulations involving graphics, computers usually have as many as 33 milliseconds of time to calculate each time step. Or when studying unique physical phenomena, computers may spend whole seconds or minutes to calculate each time step. But when synthesizing audio using virtual physics, computers have to be fast – they only have about 23 microseconds to calculate each time step, because there are 44,100 time steps per second!

This is the challenge of simulating virtual physics for synthesizing sound. Imagine simulating the sound of a string using a chain of 500 masses. Even if each mass only requires 5 multiplications per time step, the computer will need to carry out $5 \times 500 \times 44100$ multiplications per second. Yet, using such simulations an astounding array virtual physical systems can be simulated.

CCT's Berdahl is leading the effort to use Synth-A-Modeler software for meeting this challenge, all the while enabling the generation of portable and efficient program code that can be easily adjusted for precise control of detailed virtual physics simulations. Currently, applications in virtual physics for real-time systems providing auditory, visual, and haptic feedback are being studied. A repository containing more than 100 examples models has been created.

Learn more about electronic music at LSU at <http://emdm.music.lsu.edu> and digital art at LSU at <http://design.lsu.edu/art/programs/digital-art/>.

EMDM Student Work

Graduate and undergraduate students within the EMDM program are having great success in their research and performance efforts. PhD student **Danny Holmes** learned to build applications for Apple products by helping with an iOS Bootcamp at CCT. Now he has founded notnatural, LLC, his own business for apps and is working with Southern University laying the groundwork for a computer music degree.

Visit <http://notnatural.co> for more information.

LSU Hosts International Conference Celebrating Digital Music



Louisiana State University's burgeoning experimental music and digital arts programs were given a worldwide showcase by hosting the 2015 International Conference on New Interfaces for Musical Expression (NIME), the premier conference in designing human-computer interfaces and interactions for musical performance May 31- June 3, 2015. The NIME conference is truly a global event, and was held in Seoul, South Korea, and London, England in the years prior to Baton Rouge.

Organized by the LSU Center for Computation & Technology (CCT), the College of Music & Dramatic Arts (CMDA) and the College of Art & Design, NIME 2015 gathered researchers and practitioners from around the world to experience four days and nights of lectures, installations, concerts and workshops. NIME 2015 had attendees from 28 countries representing 103 separate organizations and universities. The conference included more than 100 research presentations, 27 concert pieces and 32 demonstrations, with 15 sonic art installations continuing in exhibition for the entire month of June.

R. Luke DuBois, of the Brooklyn Experimental Media Center at NYU Polytechnic, and **Sile O'Modhrain**, of the University of Michigan, were the NIME 2015 keynote speakers. Both have made significant contributions to 21st century sonic art and musical practice through their research, music, invention and art.

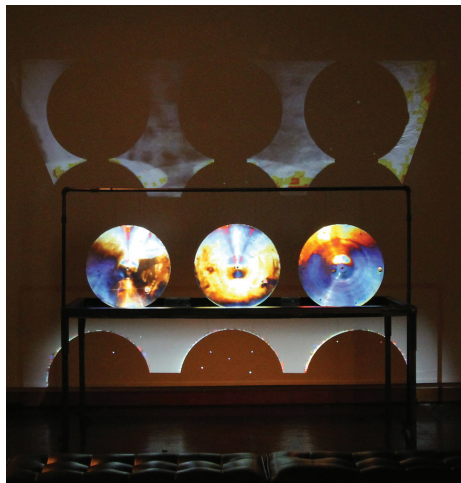
Jesse Allison, associate professor of Experimental Music & Digital Media with a joint appointment in the School of Music and the Center for Computation & Technology (CCT), chaired the 2015 conference.

"It was huge for my field to bring NIME here," Allison said. "It was a great showing of our LSU facilities, programs and students through concerts, art galleries and exhibits."

Participants got a real flavor of Baton Rouge with installations and performances across the Red Stick, including downtown art galleries, the CMDA theaters, the Shaw Center for the Arts, the Varsity Theater and LSU's Digital Media Center with state-of-the-art immersive theater including a 92-speaker array and 4K projection.

Through the tireless work of the staff of the CCT, a team of students in the EMDM and Digital Art programs, and CCT faculty **Edgar Berdahl**, **Stephen David Beck**, **Derick Ostrenko** and **Hye Yeon Nam**, the state of all things digital in Louisiana has been elevated worldwide.

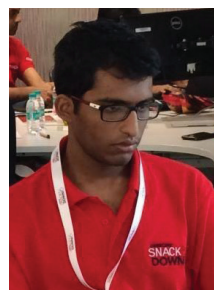
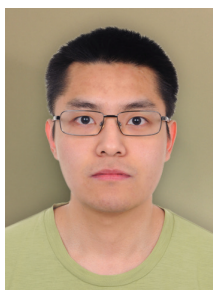
Learn more at <http://nime2015.lsu.edu>.



LSU Again Hosts Google Summer of Code Research



Google
Summer of Code



GSoC Student Participants:

Parsa Amini, Aalekh Nigam, Minh-Khanh Do and Satyaki Upadhyay

The Center for Computation & Technology's (CCT) **Systems Technology, Emergent Parallelism & Algorithm Research (STE||AR)** Group was chosen for the third year in a row as a host for Google's prestigious Summer of Code 2016 (GSoC) program.

Student developers from all over the world participate in the Summer of Code program by developing code for open source projects. In 2016, the STE||AR Group's third year to be chosen for the program, four student participants made contributions to the group's primary software product: HPX, a distributed C++ runtime system.

Student participants were **Parsa Amini**, who worked on implementation of an HPX debugger; **Aalekh Nigam**, who developed a Map/Reduce framework on top of HPX; **Minh-Khanh Do**, who extended the parallel algorithms to use a distributed data structure HPX::Vector; and **Satyaki Upadhyay**, who created a plugin mechanism for arbitrary thread schedulers in HPX.

The students who participate in GSoC gain valuable experience with real-world software development scenarios and the opportunity for potential employment. In turn, the participating hosts who will mentor students are able to easily identify and bring in new developers. Best of all, more source code is created and released for the use and benefit of everyone.

Since it began in 2005, Google Summer of Code has paired more than 12,000 student participants from 106 countries with 567

open source projects, resulting in more than 30 million lines of code. In 2016, the program accepted 178 mentoring organizations, all of which are world leaders in open-source development.

"Google's decision to continue to support our group recognizes the importance of our research in the area of distributed parallel computing," said **Hartmut Kaiser**, STE||AR Group leader at CCT and adjunct faculty in the Division of Computer Science & Engineering at LSU. "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."

J. "Ram" Ramanujam, director of CCT, said, "The STE||AR Group's work is at the leading edge of high-performance runtime systems software for high-end computing. It is an important recognition for the STE||AR Group to be selected for Google Summer of Code 2016 program, following their selection for 2014 and 2015."

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

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. More information can be found at <http://stellar.cct.lsu.edu>.

RED STICK

INTERNATIONAL FESTIVAL



Jesse Allison, associate professor of Experimental Music & Digital Media with a joint appointment with the Center for Computation & Technology (CCT), and **Randy Dannenberg**, assistant director of economic development at CCT, led both 2015 and 2016 festivals.

“Red Stick is an all-encompassing technical media arts festival,” Allison said. “It is a showcase of the investments that our state and LSU have put into digital media to bring computing and arts into the 21st century.”

The festival has a positive effect on the Baton Rouge area and Louisiana as a whole.

“Our goal with the festival is to build a mini SXSW type event. If you look at Austin 30 years ago, it was very much like Baton Rouge is today. So we see the Red Stick International Festival as an important economic development tool,” said Dannenberg. “We believe that the festival will help the tech sector in Baton Rouge, and the surrounding area, to grow and flourish.”

2015: Spotlight on LSU’s Digital Media Work, Baton Rouge and Louisiana

CCT presented the 2015 Red Stick International Festival May 29-31 in downtown Baton Rouge. More than 850 people attended the events over three days.

The 2015 Red Stick International Festival was presented in coordination with the New Interfaces for Musical Expression (NIME) conference held in Baton Rouge from May 31 – June 3, 2015. (See page 26 for more about NIME.) The symbiotic events featured an opening gala, kids’ lab, maker expo, movie and animation screenings, and art exhibitions.

R. Luke DuBois and **Evidence**, internationally renowned performers of creative sound and video art, were the headliners

of the opening gala. DuBois is well known for his internet and data-based art works, live video and sound art performance, as well as his contributions to the Jitter library for video processing.

Evidence is a collaboration between sound artists **Stephan Moore** and **Scott Smallwood**. Since 2001, they have developed a distinctive language of deeply layered sound, using field recordings of natural, urban and industrial sources as their primary material and inspiration.

The Kid’s Lab and Maker Expo at the Downtown Library included activities such as Arduino classes, classes from NIME participants open to the general public, a Showcase for some of the local school art creations. Cubee papercraft building lab, Lego lab - for created art and building lab for kids to build with Legos, and an Interactive art project on the inside of Riverside Library windows.

On Sunday May 31, the Louisiana Art and Science Museum held a screening retrospective of previous year’s Animation festivals showing selected pieces of the past RED STICK Animation festivals.

2016: Video Game Symposium and More

In 2016 the Red Stick Festival took place April 22, April 30 and May 1.

In conjunction with LSU’s Digital Media Arts & Engineering (DMAE) program, the 2016 Red Stick Festival incorporated the DMAE Video Game Symposium at the Digital Media Center (DMC) at LSU on April 22nd. Featuring video game designers from the biggest games in the world and local designers from the Baton Rouge and New Orleans areas, the summit drew more than 200 people. Red Stick’s FutureFest event featured forward-looking LSU student work in digital art, videogames and animation.



The 2015 and 2016 Red Stick festivals are part of the continuing evolution of the International Red Stick Animation Festival, which was created in 2005 by CCT's **Stephen David Beck** and **Stacey Simmons** to showcase the importance of high-performance computing through computer animation. The broader Red Stick International Festival has transitioned to include all types of digital media, including animation, maker expos, experimental music concerts, digital art exhibits, game jams, movie screenings and other technology-driven events.



Michael Blandino showing curious attendee his Wheel-O-Music - A meditative approach to creating music with the turn of a wheel.



Eric Sheffield showing off his Mechanoiser -The sounds of motors – amplified, processed and turned into music!

Photos courtesy of Red Stick International Festival

“On hand, we had **Dan Ayoub** and **Josh Holmes** who are studio leaders at 343 Industries who build Halo for Microsoft,” said **Marc Aubanel**, DMAE director. “We also had a talk by **Edward Kilham** who worked on early hits such as Star Wars TIE Fighter and Robo Sport and is now at Electronic Arts and working on FIFA. **Daniel Dociu** and **Drew Cady** who both work on Guild Wars 2 came from NC Soft. We also had guests from Heavy Iron, Nintendo, Amazon, Guild Software, Gearbox Software, Turbo Squid, High Voltage Games, InXile and Skybound Interactive. Students and local studios showed off games they have been working on over the past couple of years, and a good time was had by all.”

A complete list of symposium talks is available at <https://lsugamesymposium.cct.lsu.edu>.

The East Baton Rouge Parish Library presented several Red Stick

events on April 30. A kids' lab with interactive art exhibits was put on by the Baton Rouge Knock Knock Children's Museum partnering with LSU's College of Human Sciences and Education, LSU College of Art and Design, and CCT to transform the children's storytelling rooms of the library into a playground of light, shadows and motion. Children were delighted to use traditional materials to interact with light, color and images projected from digital devices. NASA was present with its exhibit showing what life is like for astronauts in space including a full-sized space suit and astronaut ice cream - freeze dried ice cream that NASA space travelers enjoy on the International Space Station.

Later in the afternoon, the library also hosted the Maker Expo, which included maker booths and exhibits from local companies including Electronic Arts, or EA Games; Acadian Robotics, the only 3D printer manufacturer in Louisiana; LSU's DMAE program; and members of the Maker BR group. More than 500 people came to the kids' lab and maker expo.

That evening the library hosted a screening of “Star Wars: The Force Awakens” at the main branch's event screen that included a Star Wars costume workshop for attendees.

On May 1, the Louisiana Art and Science Museum (LASM) hosted “Entangled Spaces,” a multimedia electronic music concert and live light show of experimental video and sound distributed across the LASM Planetarium by artists **Brandon Bailey**, **Matthew Blessing**, **Andrew Pfalz**, **Eric Sheffield** and **Kathy Winn** and guest collaboration with **Ken Wesley** and the DMAE program. More than 250 people attended the two live showings.

Visit redstickfestival.org for more information and follow the festival on Facebook and Twitter at @RedStickFest.

CCT and LA-SiGMA Support Research Experiences for Undergraduates, High Schoolers and Teachers



2015 REU participants and mentors

Every summer more than 150 undergraduates, high school students and teachers come to LSU from around the country to join in one of 12 unique programs designed to introduce them to the research experience. At the Center for Computation & Technology (CCT), 16 students in summer 2015 and 13 students in summer 2016 participated in the Interdisciplinary Research Experience in Computational Sciences supported by the NSF **Research Experience for Undergraduates (REU)** program.

The Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA) supported 8 additional REU students at LSU in 2015 as well as 29 REU students at other Louisiana universities. At LSU, LA-SiGMA also provided funding for seven high school students in the **Research Experience for High School Students (REHSS)** and seven teachers in the **Research Experience for Teachers (RET)** in summer 2015. These six-week programs overlap with the longer REU program. In summer 2016, two high school students in the REHSS program were supported by IBM.

CCT has hosted these programs since 2010. So far 126 undergraduates, 17 high school students and 45 teachers have completed summer research experiences at CCT. In 2016 the CCT REU program received its third grant renewal from the National Science Foundation, ensuring the program will continue for another three years.

Juana Moreno, associate professor of physics in the College of Sciences with a joint appointment at CCT, has been the principal

investigator for the NSF CCT REU grant and co-PI for the LA-SiGMA grant. **Jesse Allison**, associate professor of experimental music and digital media in the School of Music and CCT, is co-PI for the CCT REU grant. **Bety Rodriguez-Milla**, **Leigh Townsend** and **Staci Kramer** have assisted as program coordinators from 2010 to 2015, but unfortunately the coordination support was lost in summer 2016. **James Lupo**, then assistant director at CCT for computer enablement, and **Kathy Traxler**, education, outreach and training specialist at CCT, also helped with specific tasks, such as teaching Python to our students.

“The White House Computer Science for All Initiative emphasizes the great need for training workforce in computing and computational thinking,” Moreno said. *“The undergraduate and high school students participating in our program are engaged with authentic computational science projects, learn how to use state-of-the-art cyberinfrastructure tools, experience activities that characterize research careers, and work in interdisciplinary research teams. These activities have the potential to be transformative in both the students’ education as well as their future careers.”*

Olivera Dimoska, student from Florida International University, attended the 2016 CCT REU and later presented a poster of her work at the 24th Annual McNair Conference in Baltimore. After talking with other REU program students she said, *“CCT provides the best and most organized REU program among all the other REU programs from different schools. I am very grateful for being part of it and the unique experience you have provided.”*

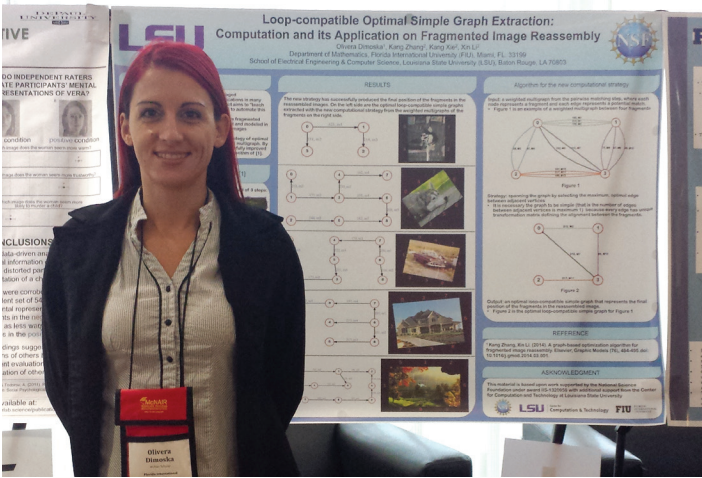
CCT’s REU program combines individual training with student immersion in a multidisciplinary research group to provide rich research experience in computation. The application process is very selective, with more than 250 applicants for the positions available each year. Students receive room and board plus a stipend, allowing them to fully focus on research.

Each participant is matched with an LSU mentor to work collaboratively on a computational research project. Student research experiences are directed by the mentors, and teachers in the RET program come to LSU with a research idea tailored to their classroom needs.

CCT REU students are included in LSU-wide REU activities, as well as a CCT-specific seminar series highlighting faculty mentors’ careers and research. At the conclusion of the REU program, students make an oral presentation in addition to



CCT REU 2016



Olivera Dimoska (CCT REU 2016) by her poster at the 24th Annual McNaair Conference in Baltimore, September 23-24, 2016.

exhibiting a poster at the **LSU Summer Undergraduate Research Forum (SURF)**. Also, they receive feedback from a visiting guest researcher. **Eric Schnetter** (Perimeter Institute for Theoretical Physics, Canada) and **Rebecca Friebrink** (Goldsmitths, University of London) were our guest researchers in 2015 and 2016, respectively.

“REU is more than just an ice breaker for students to learn about research,” Allison said. “It’s an eye opener for how they can really participate in research. We’re proud of the wide variety of students from different types of institutions who come to LSU for what can be a life-changing summer.”

More information can be found at <http://reu.cct.lsu.edu> and <http://lasigma.loni.org>.



Students from Woodlawn High School work on their robotics project.

CCT Staff Coaches Robotics Team

Frank Löffler, a research staff member at the Center for Computation & Technology, coached a 4th grade robotics team at the Westdale Heights Academic Magnet Elementary School in Baton Rouge. Within only 12 weeks, the “Blue Mind Group” learned the basics of how to design, build and program a small, LEGO-based robot, earning them an award at the final FIRST (For Inspiration and Recognition of Science and Technology) competition.

“The students learned to be gracious professionals: to learn and compete like crazy in a team but to treat one another with respect and kindness in the process, not only within their own team, but also towards their competitors,” Löffler said. “That is truly the goal of the program.”

Löffler also mentors and raises funds for the high school robotics team Panthrobotics at Woodlawn High in Baton Rouge, coached by a former CCT employee, Daniel Eiland.

Within the same robotics program, goals are set much higher here. The team of about 40 students has six weeks to build a 120-pound robot essentially from scratch. These then have to compete against robots by other teams.

In 2015, the Panthrobotics team was selected to compete in the FIRST Robotics Competition (FRC) World Championship in St. Louis, among the top 600 teams world-wide.

“Winning one of the competitions involves not only a top-performing robot but also team-spirit, outreach throughout the year, leadership and community engagement of the whole team are equally important,” Löffler said. “It is not a coincidence that FRC team members have a much higher success rate in college scholarship offers. Several Panthrobotics members received scholarship offers from LSU because of their involvement with FRC.”

CCT also provides its facilities each year for the critical kick-off of the six-week build season for FRC teams from all over Louisiana.

CCT Hosts Seventh Annual SCALA Workshop



SCALA 2015 speakers Greg Forest, Lisette de Pillis and Michele Benzi

In February 2016 the **Scientific Computing Around Louisiana**, or SCALA, workshop took place at the Louisiana Digital Media Center at LSU. The SCALA workshop focuses on cutting-edge topics in scientific computing, or using computers to examine and solve scientific problems through the analysis of mathematical models.

SCALA showcases the exciting research being undertaken at colleges and universities throughout the state and helps foster collaborations across Louisiana.

In 2016 there were about 50 participants, three invited speakers, 14 talks and 17 posters. Invited speakers were **James Nagy**, Emory University; **Carol Woodward**, Livermore National Laboratory; and **Nick Cogan**, Florida State University.

The sixth annual SCALA meeting took place at Tulane in March 2015. The invited speakers in 2015 were **Greg Forest**, University of North Carolina at Chapel Hill; **Lisette de Pillis**, Harvey Mudd College; and **Michele Benzi**, Emory University.



SCALA 2016 speakers James Nagy, Carol Woodward and Nick Cogan

Since 2010, the Center for Computation & Technology (CCT) and Tulane University's Center for Computational Science have co-sponsored SCALA and the universities alternate hosting the annual workshop. SCALA was founded and is organized by **Susanne C. Brenner**, Nicholson Professor of Mathematics at LSU and CCT Core Computational Science focus area lead, and **Lisa Fauci**, Pendergraft Nola Lee Haynes Professor of Mathematics at Tulane.

The eighth annual SCALA meeting will take place at Tulane in spring 2017.



SCALA 2016 poster session

Credit: Susanne C. Brenner

DMAE Graduate Program Approved by Board of Regents



Marc Aubanel



Ken Wesley

The Louisiana Board of Regents approved the Master of Digital Media Arts & Engineering (DMAE) Program at LSU in 2015. This is the first program of its kind in the state and joins the ranks of more than 40 successful programs around the country.

“The DMAE program’s goal is to be one of the top graduate-level interactive, media and entertainment technology programs in the world,” said **Marc Aubanel**, DMAE program director. “The digital age is bringing in large systemic changes and digital media arts is at the forefront of this revolution.”

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.

There are two full-time faculty teaching in the program, Aubanel and **Ken Wesley**. Their combined experience is more than 30 years in the feature film post-production and video game production industries; they have worked on award winning franchises such as Star Wars and FIFA Soccer.

The master’s in DMAE is a 22-month, 12-course, 45 credit-hour intensive graduate program. The courses have been designed

to ensure DMAE graduates will have the skill sets conducive to digital media and software development in the state of Louisiana and the region.

By addressing immediate industry needs where the knowledge demands on the workforce are becoming increasingly more technical in nature, the DMAE master’s program combines artistic and scientific training.

The DMAE program will train students in complex software tools such as Maya, Nuke, Unity and Houdini. “As a result, we expect the DMAE graduates to become highly sought after employees who are able to flank both the technical and creative sides while still being able to specialize,” Aubanel said.

Currently the program has seven full-time students with the first cohort graduating December 2016. The program had a total of 22 applicants and six accepted students for the Fall 2016 semester.

The master’s in DMAE is a culmination of effort that began in 2011 when a delegation from CCT went to visit the Florida Interactive Entertainment Academy at the University of Central Florida, Entertainment Technology Center at Carnegie Mellon and the University of Southern California’s Interactive Media program. Aubanel was brought on in 2013 as its founding director when the curriculum development process began.

Advisory Committee

The DMAE Advisory Committee is made up of former LSU students, faculty, and representatives from local Louisiana companies and international companies.

“Because this is a professional degree it is important that the curriculum and outcomes are vetted through an advisory committee,” Aubanel said.

Current advisory members include representatives from Electronic Arts, High Voltage, Pixel Magic, Turbosquid, Skybound and Wargaming.net.

DMAE Film Series (2014-Present)

The department holds the DMAE Film Series, which features a monthly film and a talk on a topic the DMAE field of study. The series has had the director Zaq Penn of Atari Game Over, VFX CG Supervisor Chad Wiebe of Marvel Age of Ultron, director Jeremy Snead of Making of Video Games: The Movie, and Lily Keber, the director of Bayou Maharajah. This series is free and open to the campus and helps demonstrate what leaders in the field of digital media are doing around the state and the country.



Small Things Get a Close Look at 2016 LSU NanoDays

All things tiny were on display at the seventh annual LSU NanoDays at Highland Road Park Observatory on Saturday April 16, 2016.

Children and adults were able to see how big they are compared to nanoscale objects, understand how a Scanning Probe Microscope explores the nanoworld, try to pour water out of a nano-cup, learn about nanomaterials used in stain-free clothes, have a chance to build models of nanoscale structures, play with liquid crystals and make fluids part in the middle by applying magnets to them.

Juana Moreno, associate professor at the Center for Computation & Technology (CCT) and the LSU Department of Physics and Astronomy, is the organizer of LSU NanoDays. "I have hosted NanoDays events in Baton Rouge since 2010, Moreno said. "The number of attendees has grown every year. I enlist LSU faculty, students and staff to volunteer their time to make these events a success." Every year a faculty member gives a public talk during the event.

NanoDays is a nationwide festival of educational programs about nanoscale science and engineering and its potential future impact. Each spring, NanoDays events take place at more than 250 science museums, research centers and universities across the country from Puerto Rico to Hawaii. NanoDays engages people of all ages in learning about this emerging field of science, which holds the promise of developing revolutionary materials and technologies.

In 2016, LSU NanoDays sponsors are the LSU Department of Physics and Astronomy, CCT, the LSU Department of Chemistry, the Society of Physics Students and the Consortium for Innovation in Manufacturing and Materials. CCT has been involved in NanoDays all seven years.

Learn more at www.bro.lsu.edu/programs/nano.html.



Global Game Jam at Louisiana State University 2016

The Global Game Jam (GGJ) is the world's largest game jam event (game creation). 2016 was LSU's third year as a participant in this exciting development festival, which took place January 29-31. Think of GGJ as a hackathon focused on game development. It is the growth of an idea that in today's heavily connected world we can come together, be creative, share experiences and express ourselves in a multitude of ways using video games – it is very universal.

The weekend stirs a global creative buzz in games, while at the same time exploring the process of development, be it programming, iterative design, narrative exploration or artistic expression. It is all condensed into a 48-hour development cycle. The GGJ encourages people with all kinds of backgrounds to participate and contribute to this global spread of game development and creativity.

GGJ started the afternoon of Friday January 29, 2016, with the video keynote, advice from leading game developers, and then a secret theme of "Ritual" was announced. All sites worldwide were then challenged to make games based on that same theme, with games to be completed by Sunday afternoon.

The global game jam in 2016 featured 36,000 participants from around the world, 93 countries represented with almost 6,800 games created making 2016 the largest global game jam to date.

DMAE runs the LSU chapter of the Louisiana Global Game Jam and was the sole location in the state for this year's event, and 14 games were successfully completed.

"We had more than 80 participants attend from various backgrounds including professionals, amateurs and students from around the state," **Marc Aubanel**, director of the Digital Media Arts & Engineering program, said.

LSU games completed included a Virtual Reality Beer Pong (VR Beer Pong), a training game to become the Grim Reaper where you earn your official Scythe (Grim Junior), a procedurally generated, isometric world where you nourish and destroy a forest (Inscription) and a game where users play a tomato who is struggling with identity (Ripe of Passage).

See more at <http://globalgamejam.org>.

CCT Research Staff Voluntarily Teach LSU Courses

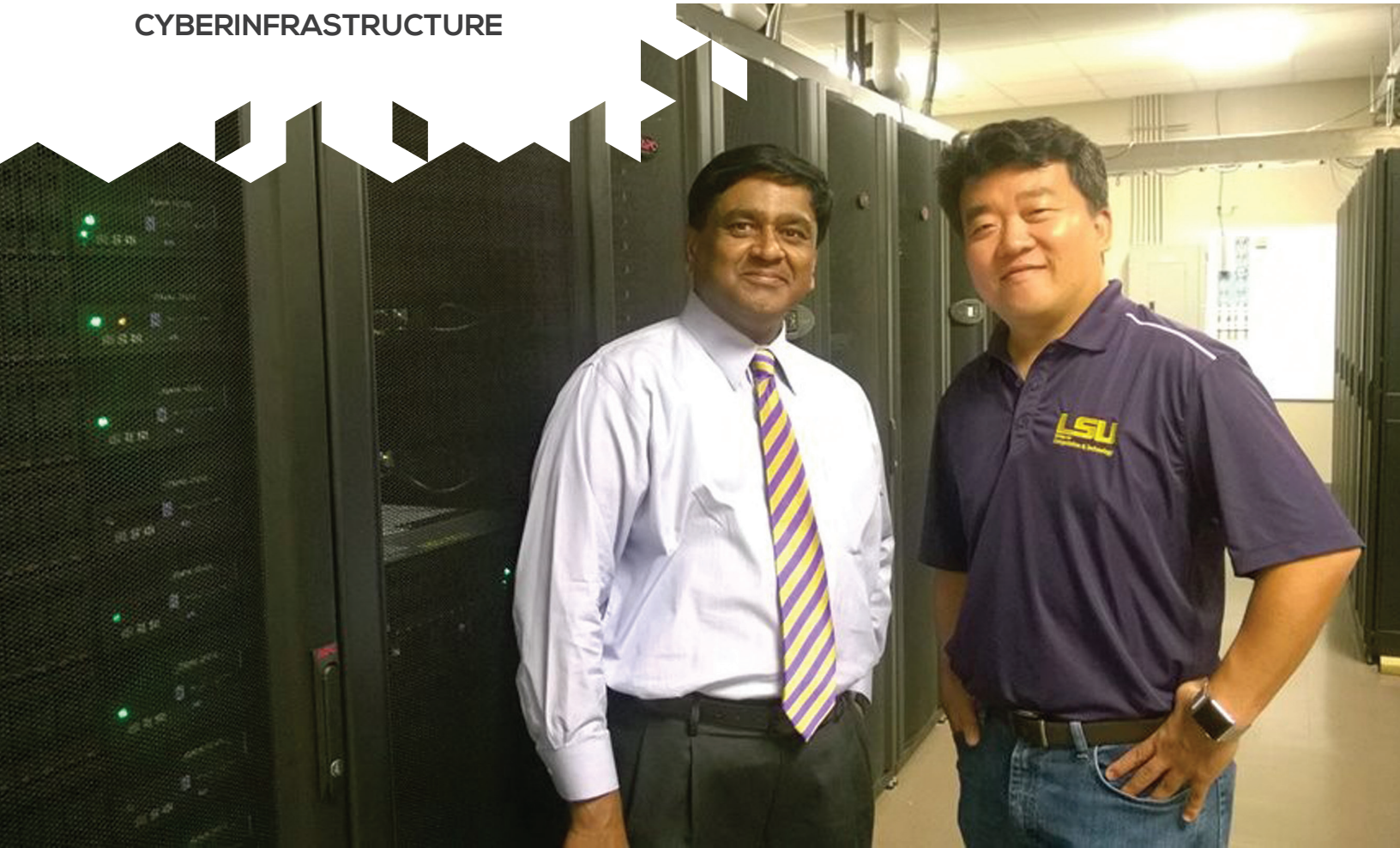
A number of research staff members at Center for Computation & Technology (CCT) voluntarily teach courses at LSU and oversee independent studies and dissertation research, mainly for the computer science and engineering division.

CLASS	INSTRUCTORS	SEMESTER
CSC1351 Computer Science II for majors (Advanced Java)	Steven R. Brandt and Frank Löffler	Spring 2015
CSC1254 Computer Science II with C++	Hartmut Kaiser	Spring 2015
CSC 4700 Scientific Programming: Python	Steven R. Brandt, Frank Löffler, and Peter Diener	Fall 2015
CSC 4585 Multicore Programming	Steven R. Brandt (with K. Busch, CSE)	Fall 2015
CSC1351 Advanced Java	Steven R. Brandt and Frank Löffler	Spring 2016
HNRS 3035 Advanced Seminar in Natural Science	Jinghua Ge (with Dominique Homberger, Biological Sciences)	Spring 2016

CCT Summer Camps

The halls of the Louisiana Digital Media Center at LSU are filled every 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 day camps for nearly 200 participants each year.

2016		2015	
May 30–June 3	Interaction Design for Music Summer Camp	June 15–19	Girls Rock – Sound Engineering Summer Camp
June 6–10	Introduction to 3D Animation Summer Camp -- Maya	June 22–26	Alice in Computation Land Summer Camp
June 13–17	Programming Music Summer Camp	July 6–10	Beowulf Boot Camp
June 20–24	PyFun Computing Summer Camp	July 13–17	Game Crash Camp
June 27–July 1	Computer Simulations Summer Camp	July 20–24	PyFun Programming for Middle School Summer Camp
July 11–15	Introduction to Video Game Creation Summer Camp: Unity	July 27–31	Programming Music Summer Camp
July 18–22	Game Crash Summer Camp		
July 18–22	Energy Venture Summer Camp		
July 25–29	Future Data Scientist Boot Camp		



CCT Deploys New IBM Supercomputer “Delta” to Advance Big Data Research in Louisiana

LSU has collaborated with IBM to deploy a powerful supercomputer to advance big data research in Louisiana. The new supercomputer has been named **Delta**, referencing both the term in the sciences used to mean “change” and the Mississippi delta region. The unique design of Delta—housed at the LSU Center for Computation & Technology (CCT)—allows a new way of conducting computational research to LSU.

LSU joins leading supercomputing agencies globally—the U.S. Department of Energy’s Oak Ridge and Lawrence Livermore National Labs and the U.K. government’s Science and Technology Facilities Council’s Hartree Centre—that have selected IBM’s POWER8 platform for cutting edge high-performance computing (HPC) research.

The IBM POWER8 processor architecture is open to development and supported by more than 150 members of the OpenPOWER Foundation, including LSU. It features a groundbreaking new

Opposite page: J. “Ram” Ramanujam and Seung-Jong “Jay” Park pose with Delta

approach to computing that uses a Coherent Accelerator Processor Interface, or CAPI, to help create powerful solutions that are highly customizable.

LSU researchers plan to utilize CAPI and tap into other innovations contributed by fellow members of the OpenPOWER Foundation to develop and implement unique algorithms to address specific data-driven challenges across a variety of science and engineering fields.

“The need for large-scale analytics in the scientific community has exploded,” said **Ravi Arimilli**, IBM Fellow and Chief Architect for Analytics and Big Data Platforms. “The POWER8 platform was designed to meet changing research needs across different domains of science.”

Arimilli is an LSU graduate in electrical engineering and in 2008 was inducted into the LSU Alumni Hall of Distinction. He has been instrumental in forging a strong partnership between LSU and IBM. The deployment of Delta is part of a series of ongoing collaborations to facilitate big data research in the state.

“Funding agencies are investing in interdisciplinary research to address the grand challenges facing society,” said **Kalliat T. Valsaraj**, LSU Vice President for Research and Economic Development. “Scientific discovery at this scale frequently requires the analysis of large volumes of data. The LSU Office of Research & Economic Development is spearheading initiatives to provide the needed resources for data-rich, interdisciplinary research at LSU and throughout Louisiana. The Delta supercomputer is an important step in that direction.”

Delta is initially being utilized to expand biomedical research capabilities in the life sciences. Delta will be equipped with the IBM Reference Architecture for Genomics, increasing scale and speed for genomics computing and enabling the development of new tools for sequencing and analysis.

“LSU is a leader in biomedical research, which is an important economic driver for the state,” said **Gus Kousoulas**, associate vice president for research and economic development at LSU. “Computational biology and bioinformatics have become linchpins for progress in biomedical and biotechnology research. Delta will enable quantitative analysis and interpretation of large biological genomics data generated at LSU.”

In addition to bioinformatics and computational biology, computer scientists at IBM and CCT are working with LSU researchers in the coastal sciences. Delta will enable the integration of vast quantities of heterogeneous environmental data and the development of analytics tools and computational models essential to improving the sustainability and resilience of sensitive coastal environments.

CCT Director **J. “Ram” Ramanujam** said, “CCT is making targeted investments in data analytics—computing and storage resources and personnel—to enable a variety of research endeavors LSU-wide. We expect significant growth in new areas of research including bioinformatics, systems biology, health data analytics and cyber security.”

Delta has been designed to continue expanding the platform’s capabilities and to meet the changing needs of the science community.

“The new research capabilities offered by the IBM Delta supercomputer represent a tremendous opportunity for LSU researchers,” said LSU President **F. King Alexander**. “We look forward to continuing our collaboration, which benefits not only our university and IBM, but the entire state of Louisiana.”



LSU Team Receives I-Corps Grant to Commercialize 3D Printer Accuracy Technology

As the importance of technology transfer of university research into the marketplace continues to grow, the National Science Foundation is taking steps to assist researchers on their journeys from lab to market. The NSF Innovation Corps (I-Corps) program is designed with a primary goal to foster entrepreneurship that will lead to the commercialization of technology that has been supported previously by NSF-funded research.

Chris Branton, then IT consultant at CCT and adjunct professor in LSU's Department of Computer Science & Engineering, is principal investigator of an I-Corps team that received a \$50,000 grant in 2015. (As of August 2016, Branton is an assistant professor of computer science at Drury University in Missouri.)

Along with entrepreneurial lead and LSU student **Gerry Knapp** and business mentor **Larry Simeral**, visiting professor in LSU's Department of Chemistry and retired distinguished adviser at the Albermarle Corporation, the team studied the commercial viability of a 3D printing quality analysis product. Knapp is one of only a handful of undergraduate student entrepreneurial leads to be part of the national I-Corps Teams program.

In summer 2015 the team took part in an intensive seven-week process to determine whether a market exists for their technology, which compares the design of a 3D-printed object to a scan of the final object to determine differences and tweaks needed to improve quality.

The focus of I-Corps work is to determine who the potential

customers are and what the team can give them, Branton said. The team's idea developed from research being done by **Les Butler**, LSU chemistry professor and adjunct faculty member at CCT.

During their work the team found there are two basic types of 3D printer users: hobbyists or makers and advanced manufacturers. Branton said the makers generally are satisfied if the final product is sufficiently close to the design, and advanced manufacturers need to be able to predict the product's quality before it is printed.

Ultimately the team discovered that their product idea is part of a bigger project yet to be created, Branton said.

"At the end of the I-Corps experience you come to one of three next steps," Branton said. "The product is ready to develop, it needs to go back to the lab or it should be dropped. We think we found a viable business model, but it's not exactly the product we came to the program with. This is a work in progress."

Branton said the I-Corps program is very valuable.

"I-Corps has really changed the way I approach research and teaching," he said. "I'd do it again in a heartbeat. I'll definitely apply what I learned to future ideas."

Simeral agreed. "The experience provided the team with a good overall business start-up experience based on a scientific approach," he said. "It was a challenging and exciting experience."

Opposite page: Larry Simeral, Gerry Knapp and Chris Branton

Knapp, who graduated in May 2016 with a degree in mechanical engineering, said the I-Corps experience was worthwhile and challenging.

"I learned a lot more than I have at any other summer program that I've done," Knapp said. "The program was very beneficial to me because now when I go to graduate school I'll be able to apply a lot of what I learned to my future research."

In January 2016, LSU was named an I-Corps Site, which will provide entrepreneurial training and develop more future I-Corps

teams. **Andrew Maas**, director of the Office of Innovation & Technology Commercialization, leads the LSU site.

The LSU I-Corps Site's goal is to strengthen the pipeline of faculty, students and community members who can feed into the Louisiana Business & Technology Center and be more competitive for LSU Leveraging Innovation for Technology Transfer, or LIFT2, grants; the NSF I-Corps Teams program; and national Small Business Innovation Research (SBIR) agency programs.

Learn more at www.lsu.edu/innovation/ICorps.

CCT Researchers Win LIFT2 Technology Transfer Grant



Mayur Sathe



Krishnaswamy Nandakumar

Center for Computation & Technology (CCT) researcher **Mayur Sathe** leads one of the 15 innovative projects developed by LSU system faculty that received funding through the LIFT2, or Leverage Innovation for Technology Transfer, fund in October 2015. The project, "Space filling high-throughput microbubble generator," is led by Sathe and **Krishnaswamy Nandakumar**, adjunct faculty at CCT and professor in the LSU Cain Department of Chemical Engineering.

The LSU Board of Supervisors created the LSU LIFT2 program to provide support to help transfer LSU technologies and innovations to the market – support that is difficult to come by through traditional means. Providing a bridge over the critical gap between basic research and commercialization, the LSU LIFT2 Fund awards grants to faculty on a competitive basis twice a year, in amounts up to \$50,000, to validate the market potential of their inventions. Nearly \$530,000 was awarded in 2015 to the proof-of-concept projects from a portion of the licensing income generated by previous inventions created at the university.

By permanently securing a portion of licensing income for the LSU LIFT2 Fund, LSU has ensured continual reinvestment in new innovation opportunities and affirmed its commitment to advancing discoveries for public benefit. Commercialization of academic innovations through technology transfer further enhances multiple aspects of LSU's mission and creates new economic opportunity in Louisiana and elsewhere.

Inventorship Showcase

Sathe displayed his microbubble generator, funded by the LIFT2 grant, at the second annual Inventorship Showcase held at the Lod Cook Alumni Center on the LSU campus on April 19, 2016. "We are displaying a microbubble generator and what it does is it disperses a large amount of gas into a big pool of liquid," Sathe said. "So what we can make with this device is a small enough bioreactor that fits on a utility truck." He hopes to have his generator used by companies looking for alternatives to their bioreactors. He said he's already received interest from the waste production facility LanzaTech.

Many researchers at LSU had the opportunity to display their inventions during the two-hour event. The event drew around 150 participants in 2016 – an increase of 30 from the previous year.

LSU Director of Innovation and Technology Commercialization **Andrew Maas**, who organized the event, said, "One of the main motivations behind this event is to recognize our faculty for the great things they do in innovation and to put them in a situation where they can rub shoulders with industry partners that are interested in their technology."



2015 LSU Rainmaker recipients with LSU leaders

Credit: Eddy Perez, LSU

CCT's Allison Honored with LSU Rainmaker Emerging Scholar Award

Jesse Allison, associate professor of Experimental Music & Digital Media with a joint appointment in the School of Music and CCT, was named a 2015 LSU Rainmaker, receiving the Arts, Humanities, Social & Behavioral Sciences Emerging Scholar award.

Allison, a member of CCT's Cultural Computing focus area, is a leader and innovator in sonic art technology. His research and invention interests focus on computer interactivity in performance, distributed music systems, mobile music, interactive sonic art installations, hybrid world experiences and multimodal artworks.

"I've been developing ground breaking distributed performance art works, creating a hub for communications and coordinating many users in performance," Allison said. CCT has supported Allison's work by providing shared resources in digital fabrication, recording facilities, and assistance in the creation of the unique HPC, HIVE which enables real-time supercomputing for artistic endeavors.

The NexusUI toolkit, a very successful open-source Javascript library for browser-based user interaction, was developed from Allison's research in distributed performance systems. NexusUI enables large-scale collaborative performances using cell phones, and as of December 2014 had more than 11,000 unique users. (See <http://nexusosc.com> for more.)

"Since his arrival in 2010, Jesse has been active in promoting the integration of STEM with sonic arts and CCT," said J. "Ram" Ramanujam, CCT director. His outreach has involved collaborations with the LASM, EBR Public Library, Redstick Festival, a number of EBR Parish Schools including a recent collaboration with Lee Magnet High School in developing their forward-looking digital arts curriculum.

Allison is the coordinator of the LSU Experimental Music & Digital Media program in the School of Music, co-directs the Laptop Orchestra of Louisiana, is co-PI on the NSF funded REU program in computational science, and chaired the 2015 International Conference on New Interfaces for Musical

Expression at LSU (see page 26).

The LSU Office of Research & Economic Development, with the support of Campus Federal Credit Union, annually honors a few outstanding LSU faculty members with the Rainmaker Awards for Research and Creative Activity.

Rainmakers are faculty members who balance their teaching and research responsibilities while extending the impact of their work to the world beyond academia. These outstanding faculty members also have established track records in securing external research funding and publishing in high-impact journals.

"We acknowledge the talent and dedication among LSU faculty

by recognizing these exemplary individuals as Rainmakers. They are part of what makes this university great," said **Kalliat T. Valsaraj**, Vice President of Research & Economic Development at LSU.

The Rainmaker awards have been presented since 2010. In that time four CCT faculty members, Jesse Allison (2015), Hongchao Zhang (2013), Rudy Hirschheim (2012) and Bijaya Karki (2010) have been honored in addition to two adjunct faculty members at CCT: Francisco Hung (2014) and Parampreet Singh (2014).

For more information about the Rainmaker awards and a list of other honorees see www.lsu.edu/research/research/council_on_research/rainmaker.php

CCT's Brenner Named Nicholson Professor



Susanne C. Brenner

Susanne C. Brenner was named the Nicholson Professor of Mathematics at Louisiana State University in 2015. Brenner holds a joint appointment with the Department of Mathematics and the Center for Computation & Technology (CCT). At CCT she has served as the associate director for academic affairs since 2008. Previously she was the Michael F. and Roberta Nesbit McDonald Professor of Mathematics.

"We are fortunate to have a preeminent scholar, Sue Brenner, as our colleague at LSU in the Department of Mathematics and as a leader at CCT," said **Cynthia Peterson**, dean of the College of Science. "Dr. Brenner is an exemplary faculty member and internationally recognized researcher who is highly deserving of the prestigious Nicholson Professorship."

Robert Perlis, chair of the LSU math department at the time of the announcement, said, "Sue Brenner has an international reputation as a leader in the field of numerical analysis. The Nicholson Professorship recognizes her prominence as a researcher and expositor."

The Nicholson Professorship of Mathematics is among the highest professorial ranks awarded by the university. Faculty members who are designated as Nicholson professors have attained both national and international distinction for outstanding teaching, research or other creative achievement.

The professorship was established in memory of former professor and university President James William Nicholson. Nicholson served LSU in many capacities from 1873 until his death in 1917. His first professional interest was in mathematics, and his association with the math department continued throughout his 44 years of service to the university.

Hui-Hsiung Kuo, professor emeritus, previously held the Nicholson professorship.

Pullin Named LSU Distinguished Research Master



Jorge Pullin with K.T. Valsaraj (LSU Vice President of Research & Economic Development) and Cynthia Peterson (Dean, College of Science)



Credit: Eddy Perez, LSU

The Center for Computation & Technology's **Jorge Pullin**, Horace Hearne Jr. Chair in Theoretical Physics at LSU, was selected as a 2014 Distinguished Research Master in May 2015. Presented by the LSU Office of Research & Economic Development (ORED), the honor recognizes exceptional achievements in research and scholarship.

Pullin is also the co-director of the Horace Hearne Jr. Institute for Theoretical Physics and served as interim CCT director in 2014. He holds a joint appointment in the LSU Department of Physics & Astronomy and CCT.

Pullin received his Ph.D. in physics from the Instituto Balseiro in Bariloche, Argentina, in 1989. He has held academic positions at the University of Cordoba in Argentina, Syracuse University, the University of Utah and Penn State.

"It is great to be recognized by LSU, an institution with a great collegial atmosphere I love being a part of," Pullin said.

His research is in the area of classical and quantum aspects of general relativity and gravitation, particularly in an approach known as loop quantum gravity, of which he is one of the earlier contributors. The National Science Foundation has continuously supported his work.

He is the coauthor of two books, published by Cambridge and Oxford University presses, including the only book for undergraduates about loop quantum gravity, which has been translated into Spanish and Japanese. He received the Edward Bouchet award of the American Physical Society and is a fellow of the American Physical Society and the American Association for the Advancement of Science. He is a fellow and Chartered Physicist of The Institute of Physics and a member of the National Academies of Mexico and Argentina and the Latin American Academy of Sciences. He serves on the editorial board of several journals and is the founding editor of *Physical Review X*, published by the American Physical Society, the second most impactful journal covering all of physics. He was a Fulbright, Alfred P. Sloan and John S. Guggenheim fellow.

The Distinguished Research Master awards have been presented since 1972. Recipients receive a salary stipend and the University Medal – the symbol of exceptional academic accomplishment at LSU. Past recipients with joint faculty appointments at CCT include Nicholson Professor Susanne C. Brenner (2013), Director emeritus Joel Tohline (2000) and S.S. Iyengar, Professor Emeritus (1998).

Walker Receives the NSF CAREER Award



Shawn W. Walker



Students interact with liquid crystals during Sit-with-a-Scientist program at the East Baton Rouge Parish Public Library in summer 2016.

Shawn W. Walker, associate professor of mathematics and faculty member in the Center for Computation and Technology (CCT), has been awarded a five-year Faculty Early Career Development, or CAREER, grant from the National Science Foundation.

The CAREER award is one of NSF's most prestigious grants given to promising junior faculty who effectively integrate research and education within the context of the mission of their organization. Walker has received a \$400,000 award to support his research proposal, Numerical Methods for Liquid Crystals and Their Optimal Design, from August 2016 through July 2021.

Liquid crystals are commonplace in modern technological devices, and are most famously used for their optical properties in electronic displays.

The goal of Walker's research project is to create new mathematical methods or algorithms for simulating liquid crystal phenomena and for designing new materials that utilize liquid crystals. In other words, the research will provide the groundwork for developing functionalized and switchable materials that are "driven" by liquid crystal physics.

"This research will build on liquid crystal physics, the same technology in your LCD screens, with a focus on laying the groundwork to create novel materials," Walker said. "I will share my work with middle and high school students and encourage their pursuit of STEM careers through a 'sit-with-a-scientist' program to be launched at East Baton Rouge Public Library branches."

Each sit-with-a-scientist program will take place at a library

branch and include a short, introductory presentation followed by hands-on activities to allow the students to actively learn about the physics and mathematics of liquid crystals. Walker will also mentor middle school students' science fair projects and work with graduate students and post-docs. As part of his work, Walker has created a video showing the mathematical modeling of liquid crystals set to music, which you can see at http://youtu.be/pWWw7_6cQ-U.

Cynthia Peterson, College of Science dean and Seola Arnaud and **Richard Vernon Edwards Jr. Professor**, said, "This award is a testament to the caliber of young faculty we have in the college and their impact on LSU's research footprint. On behalf of the LSU College of Science, I congratulate Dr. Walker on receiving such a distinguished honor."

J. "Ram" Ramanujam, director of CCT, said, "Shawn is a first-class applied mathematician and computational scientist. He has done seminal work on the development of numerical methods for shape optimization. His work successfully integrates mathematical analysis, modeling and algorithm development. Shawn highly deserves this recognition."

Walker's research interests include partial differential equations for multi-physics problems, geometric evolution and free boundary problems, numerical analysis/finite element methods and mesh generation. He has authored or coauthored more than 20 publications in his field and wrote a book, "The Shapes of Things: A Practical Guide to Differential Geometry and the Shape Derivative."

Oak Ridge Associated Universities Honors CCT Faculty Members



Ken Lopata

Two faculty members from Center for Computation & Technology (CCT) were honored with Oak Ridge Associated Universities' (ORAU) Ralph E. Powe Junior Faculty Enhancement Awards in 2015.

Celalettin Emre Ozdemir, assistant professor in the Department of Civil & Environmental Engineering, and **Ken Lopata**, assistant professor in the Department of Chemistry, received grants for the 2015-16 academic year.

Ozdemir studies marsh erosion and other sediment transport processes in the Gulf Coast. This award supports his new research effort to build multi-scale erosion models that will advance our understanding of and the ability to predict marsh erosion at a large range of length scales (from centimeters to kilometers).

"My new research has the potential to help people living on coastlines that are threatened by coastal erosion including those who live in Louisiana," Ozdemir said. "This award gives me tremendous motivation to pursue this project, which may become an overarching component of my career."

Lopata has been developing computational simulations of the response of electrons and nuclei in insulating materials when subjected to very intense light; this is crucial for interpreting and motivating cutting-edge experiments, and ultimately for designing tunable electromagnetically hardened materials.

He will use the award to buy a computer system to develop the required prototype software for the project. He will then scale-up the computer simulations to high-end supercomputers at LSU and at different computing facilities operated by the Department of Energy and the National Science Foundation around the country.

"This award gives me the computational resources necessary to develop code that will ultimately run on some of the largest supercomputers in the world," Lopata said.

Given to junior faculty at ORAU-member institutions, Ralph E. Powe awards provide research seed money to enrich recipients' research and professional growth and result in new funding opportunities. See www.ornl.gov/university-partnerships/faculty-student-programs/powe for details.

Previous awardees at CCT include joint faculty member Michal Brylinski (2012) and adjunct faculty member Francisco Hung (2008).



Celalettin Emre Ozdemir

Notable Publications

◇ **Susanne C. Brenner**, Nicholson Professor of Mathematics at LSU and CCT Core Computational Science focus area lead, edited “Topics in Numerical Partial Differential Equations and Scientific Computing,” published in 2016 by The IMA Volumes in Mathematics and its Applications. The book is based on the research initiated at the IMA’s WhAM! A Research Collaboration Workshop for Women in Applied Mathematics that took place August 12-15, 2014, and was organized by Brenner.

Brenner’s book “The mathematical theory of finite element methods” has been cited more than 6,300 times so far, according to Google Scholar.

◇ **Michal Brylinski**, assistant professor in Biological Sciences and CCT (along with Yun Ding, Ye Fang, Wei Feinstein, J. “Ram” Ramanujam, D. Koppelman, J. Moreno and M. Jarrell), published the article “GeauxDock: A novel approach for mixed-resolution ligand docking using a descriptor-based force field” in the Journal of Computational Chemistry (vol. 36, no. 27, pages 2013-2026) in 2015. The editors of the Journal of Computational Chemistry selected this paper for the front cover because it is well suited for proteome-scale applications utilizing the increasingly growing protein sequence and structural data.

Brylinski had another article, “eMatchSite: Sequence Order-Independent Structure Alignments of Ligand Binding Pockets in Protein Models,” selected by the editors of PLoS Computational Biology for the front cover due to its remarkable potential for polypharmacology and rational drug repositioning.

◇ **Rudy Hirschheim**, professor at CCT and the Ourso Family Distinguished Professor of Information Systems, has been ranked internationally at the top of his field previously by two separate studies. In 2010, a study (authored by Lin and Gregor) that ranked the productivity of information systems researchers from around the world using the top six journals in the field, ranked Hirschheim second in the world. Another study used the Hirsch family of indices to evaluate research influence and looked at more than 4,000 candidates, ranked Hirschheim among the top 10 to 15 researchers in the world in information systems. Hirschheim has published seven articles that have each been cited more than 500 times, according to Google Scholar. To date, his publications have been cited more than 19,200 times.

◇ “The Shapes of Things: A Practical Guide to Differential Geometry and the Shape Derivative,” a book on differential geometry by **Shawn W. Walker**, associate professor in the Department of Mathematics and CCT, was published by the Society for Industrial and Applied Mathematics (SIAM) in 2015. “The Shapes of Things,” a reference book for students and scientists using surface geometry and shape optimization in their work, was derived from lecture notes Walker created and refined while teaching a special topics course at LSU in 2011.

◇ **Mark M. Wilde**, assistant professor in Physics & Astronomy and CCT, proved a physically meaningful enhancement of a 40-year-old theorem known as the quantum data processing inequality, which underlies nearly all the communication bounds of quantum information theory. The article “Recoverability in quantum information theory” appears in the Proceedings of the Royal Society A. He has now applied this theorem in a variety of contexts, to sharpen the uncertainty principle of quantum mechanics, the second law of thermodynamics and the no-cloning theorem of quantum information.

Honors and Awards

Jesse Allison

- ◇ 2015 LSU Rainmakers Emerging Scholar Award

Susanne C. Brenner

- ◇ Nicholson Professor of Mathematics, LSU (2015-present)
- ◇ Infosys Visiting Chair Professor, Indian Institute of Science (2015-2020)
- ◇ Advisory Committee for Mathematical and Physical Sciences, National Science Foundation, (2016-present)
- ◇ Scientific Council, Centre International de Mathématiques Pures et Appliquées (CIMPA) (2009-present)
- ◇ Scientific Council, Société de Mathématiques Appliquées et Industrielles (SMAI) (2014-present)

Scott Hagen

- ◇ Inducted into the University of Iowa Distinguished Engineering Alumni Academy

Robert Kooima

- ◇ Tiger Athletic Foundation (TAF) Undergraduate Teaching Award

Revati Kumar

- ◇ Tiger Athletic Foundation (TAF) Undergraduate Teaching Award

Ken Lopata

- ◇ Oak Ridge Associated Universities' Ralph E. Powe Junior Faculty Enhancement Award

Celalettin Emre Ozdemir

- ◇ Oak Ridge Associated Universities' Ralph E. Powe Junior Faculty Enhancement Award
- ◇ Enhancement Award

Seung-Jong "Jay" Park

- ◇ IBM Faculty Award

Gabriele Piccolli

- ◇ Best Information Systems Publication Award (2015) for the article: "Impact of Mobility and Timing on User-Generated Content"

Jorge C. Pullin

- ◇ LSU Distinguished Research Master 2015
- ◇ Delivered a public lecture and a departmental colloquium at the Instituto de Física y Matemáticas Universidad Michoacana de San Nicolás de Hidalgo in Morelia, Mexico, as part of their celebrations of the 100 years since Einstein presented his general theory of relativity.
- ◇ Named Fellow of the International Society on General Relativity and Gravitation for "his outstanding contributions to loop quantum gravity, black hole binaries, and the foundations of quantum mechanics and for his service within the U.S. and international relativity community." Pullin joins an induction class of physicists that includes Stephen Hawking.

Mayank Tyagi

- ◇ IBM Faculty Award

Shawn W. Walker

- ◇ 2016 NSF CAREER Award
- ◇ 2016 LSU Alumni Association Rising Faculty Research Award

R. Clint Whaley

- ◇ IBM Faculty Award

Mark M. Wilde

- ◇ 2016 LSU Alumni Association Rising Faculty Research Award

Hongchao Zhang

- ◇ McGehee Award for Excellent Research by a Junior Faculty Member

Adjunct Faculty:

Francisco Hung

- ◇ 2014 LSU Rainmakers Emerging Scholar Award

Parampreet Singh

- ◇ 2014 LSU Rainmakers Emerging Scholar Award

New Hires

Scott Hagen joined as professor in the Department of Civil and Environmental Engineering and CCT in January 2015. In addition, he is the director of the LSU Center for Coastal Resiliency. He came to LSU from the University of Central Florida.

Giulio Mariotti joined the Department of Oceanography & Coastal Sciences and CCT in January 2015. He was previously a W.O. Crosby Postdoctoral Fellow at the Massachusetts Institute of Technology's Department of Earth, Atmospheric, and Planetary Sciences.

Seungwon Yang started as Assistant Professor in the School of Library and Information Sciences and CCT in August 2015. He received a Ph.D. in Computer Science from Virginia Tech in 2013 and was a postdoc at George Mason University, before coming to LSU.

Erica W. D'Spain joined the center as Manager of Grants and Contracts in July 2015.

Nicolas Loup started as Purchasing Coordinator in October 2015.

Faculty Promotions

Theda Daniels-Race: Promoted to Professor, Electrical and Computer Engineering Division, effective, August 2015

Xiaoliang Wan: Promoted to Associate Professor with tenure, Mathematics, effective August 2015

Shawn W. Walker: Promoted to Associate Professor with tenure, Mathematics, effective August 2016

Jesse Allison: Promoted to Associate Professor with tenure, School of Music, effective August 2016

Seung-Jong "Jay" Park: Appointed as Associate Director for Data Science & Cyberinfrastructure, CCT, effective January 2016; Promoted to Professor, Computer Science and Engineering Division, effective August 2016

LSU Distinguished Research Master Awards

Jorge Pullin (2014)
Susanne C. Brenner (2013)
Joel Tohline (2000), Director Emeritus
S.S. Iyengar (1998), Professor Emeritus

LSU Rainmaker Awards (2010-present)

Jesse Allison (2015)
Hongchao Zhang (2013)
Rudy Hirschheim (2012)
Bijaya Karki (2010)
Francisco Hung (2014), adjunct faculty; currently at Northeastern University
Parampreet Singh (2014), adjunct faculty

National Science Foundation CAREER Awards

Shawn W. Walker
Mark M. Wilde
Georgios Veronis
R. Clint Whaley
Juana Moreno
Q. Jim Chen
Bijaya Karki
Tevfik Kosar (currently at University at Buffalo-SUNY)
Jorge Pullin
Francisco Hung (adjunct faculty; currently at Northeastern University)
Parampreet Singh (adjunct faculty)

National Science Foundation Young Investigator Awards

J. "Ram" Ramanujam

CCT-Sponsored Conferences and Events: Spring 2015-Summer 2016

2016

LSU Center for Coastal Resiliency - Kickoff Symposium
August 16, 2016

CCT Future Data Scientists Summer Camp
July 25 - 29, 2016

SURF (Summer Undergraduate Research Forum)
July 11-15, 2016

IBM Workshop & Training
May 30 - June 3, 2016

NVIDIA GPU Workshop
June 1-2, 2016

**5th Annual LONI HPC (Louisiana Optical Network Initiative
High Performance Computing) Parallel Programming Workshop**
May 30-31, 2016

Red Stick Festival
April 30 - May 1, 2016

Imaging Symposium: Biomedical, Materials & Computation
April 23, 2016

Red Stick Future Fest
April 22, 2016

LSU Video Game Symposium
April 22, 2016

IGL (Independent Gaming League) Indie Game Tournament
April 20, 2016

**DMAE (Digital Media Arts & Engineering) Film Screening of
"Run Lola Run"**
April 6, 2016

**4th Annual LA Conference on Computational Biology &
Bioinformatics**
March 9, 2016

PC4G (Programming Challenge for Girls) 2016
March 1, 2016

**Introduction to OpenFOAM (Open-source Field Operation And
Manipulation)**
February 24, 2016

DMAE Film Screening of "Spirited Away"
February 17, 2016

SCALA (Scientific Computing Around Louisiana) Workshop
February 3, 2016

Global Game Jam at Louisiana State University 2016
January 29-31, 2016

DMAE Film Screening of "Atari: Game Over"
January 27, 2016

Cinema for the Ears Concert
January 25, 2016

2015

CCT at SC15 (Supercomputing 2015) in Austin, Booth #1233
November 16-19, 2015

DMAE Film Screening - 3 Short Films
November 16, 2015

WICS (Women In Computer Science) Game Jam
November 6-8, 2015

ACM ICPC (Association for Computing Machinery International Collegiate Programming Contest) South Central USA Regional Programming Contest
November 6-7, 2015

DMAE Movie & Student Recruitment: "Avengers Age of Ultron"
October 26, 2015

Digital Divide: Performance by Jesse Allison
September 24, 2015

DMAE Film Night: "Ex_Machina"
September 14, 2015

Katrina & Rita Symposium
August 28, 2015

Science Visualization Training
August 24-25, 2015

Supercomputing for Everyone Training
August 17-21, 2015

Red Stick Festival Outdoor Screening of "Pitch Perfect"
August 15, 2015

SURF (Summer Undergraduate Research Forum)
July 31, 2015

DMAE Film Series: Game Over: Rise of the Indies (2015)
June 24, 2015

Intel Xeon Phi Workshop
June 4, 2015

NIME (New Interfaces for Musical Expression) Conference
May 31-June 3, 2015

LONI HPC Parallel Programming Workshop
June 1-3, 2015

Red Stick International Festival 2015
May 29-31, 2015

3rd Annual EPIC (Enabling Process Innovation through Computation) Workshop
May 1, 2015

LA Conference on Computational Biology & Bioinformatics
April 17-18, 2015

SCALA (Scientific Computing Around Louisiana) 2015
March 20-21, 2015

CCT Computing & Math Saturdays for High School Students
March 14, 2015

CCT at GDC (Game Developers Conference), Booth #cc3300
March 4-6, 2015

High Harmonic Spectroscopy Workshop
March 2-3, 2015

Workshop: A Focus on Biotechnology
February 27, 2015

LSU Cinema for the Ears Concert
February 23, 2015

20th Mardi Gras Conference "Petascale Many-Body Methods for Complex Correlated Systems"
February 12-14, 2015

CCT at PAX (Penny Arcade Expo) South, Booth #1643
January 23-25, 2015

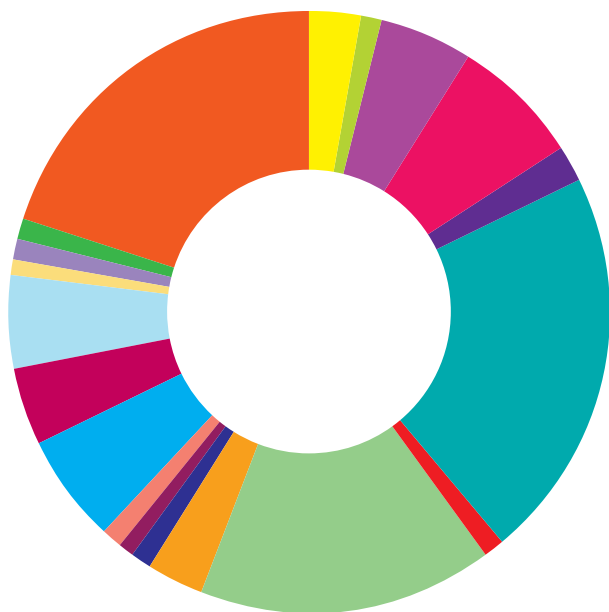
Business Reports

CCT Faculty by Department



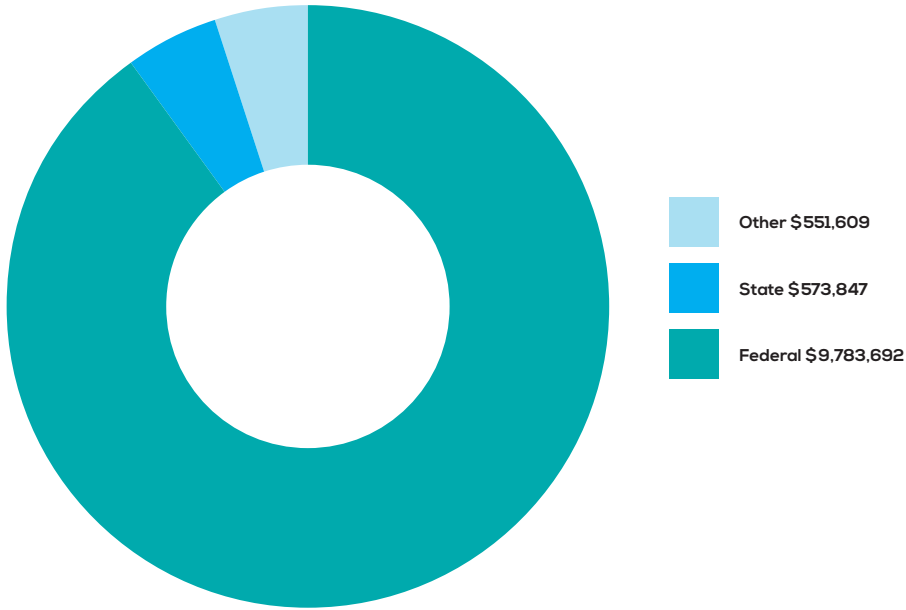
- Physics & Astronomy 13%
- Petroleum Engineering 3%
- Oceanography & Coastal Studies 8%
- Music 8%
- Mathematics 10%
- Mass Communication 3%
- Library & Information Science 3%
- Information Systems & Decision Science 5%
- Electrical & Computer Engineering 10%
- Computer Science & Engineering 13%
- Civil & Environmental Engineering 8%
- Chemistry 5%
- Chemical Engineering 3%
- CCT 5%
- Biological Sciences 3%
- Art & Design 3%

CCT Graduate Assistants by Department

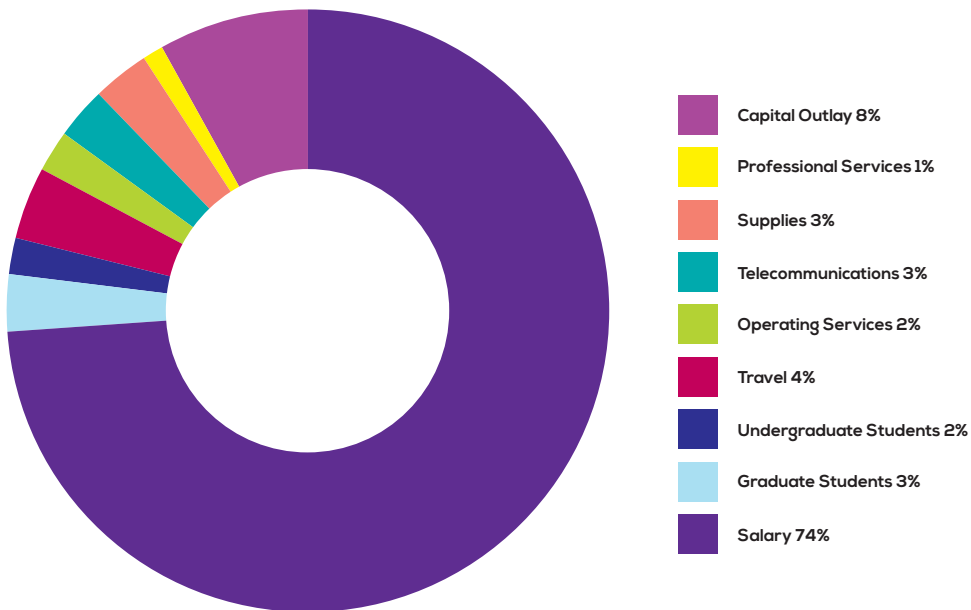


- Physics & Astronomy 20%
- Petroleum Engineering 1%
- Oceanography & Coastal Studies 1%
- Natural Sciences 1%
- Music 5%
- Mechanical & Industrial Engineering 4%
- Mathematics 6%
- Library & Information Sciences 1%
- History 1%
- Geology & Geophysics 1%
- English 3%
- Electrical & Computer Engineering 16%
- Education 1%
- Computer Science 21%
- Civil & Environmental Engineering 2%
- Chemistry 7%
- Chemical Engineering 5%
- Biological & Agricultural Engineering 1%
- Art 3%

Total New External Funding by Source (2015-16)



CCT Investment Summary



LSU