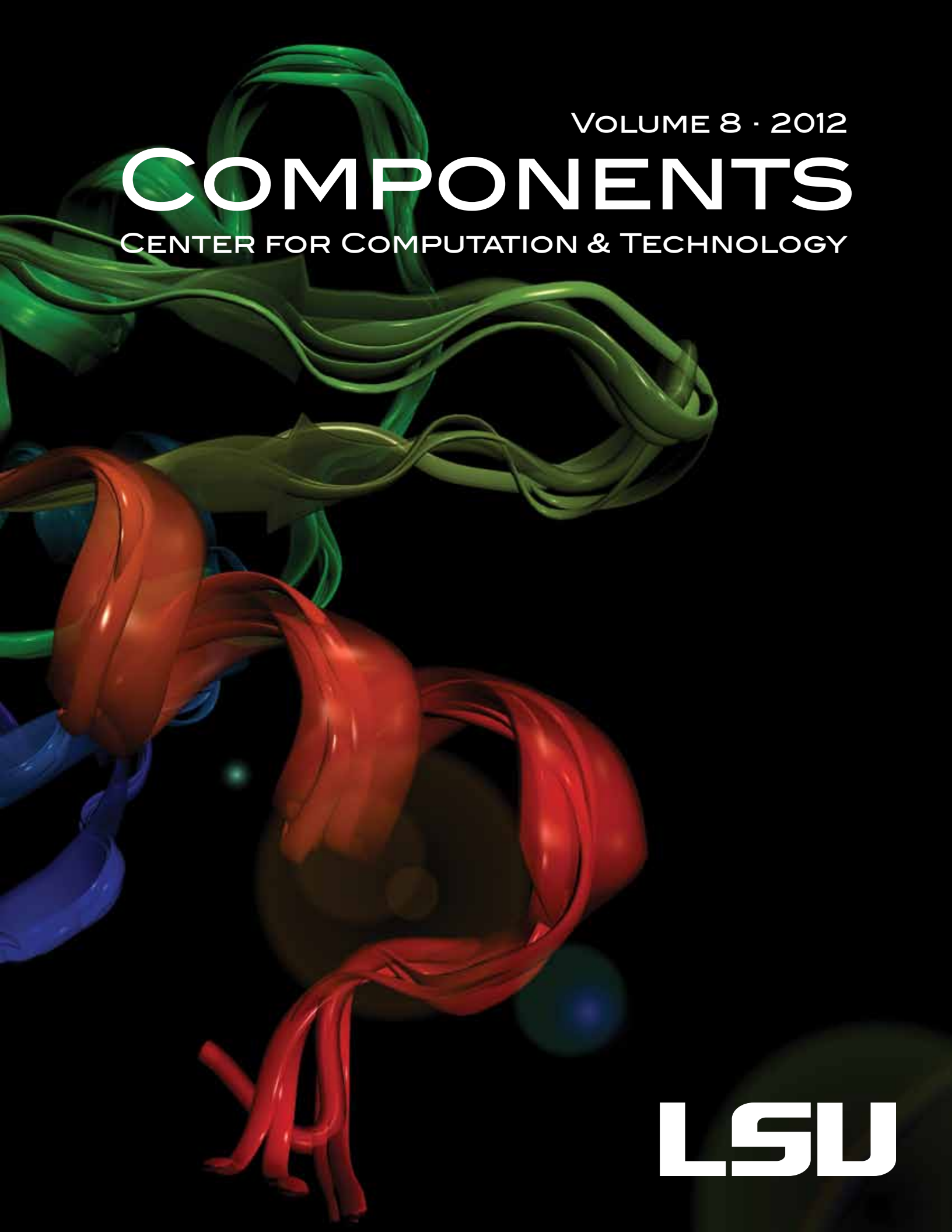

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Components

Center for Computation & Technology

LSU

LSU CENTER FOR COMPUTATION & TECHNOLOGY

Components
Volume 8

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The LSU Center for Computation & Technology is an interdisciplinary research center that advances the University's Flagship Agenda and promotes economic development for the state by using computational science 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 the CCT use the advanced cyberinfrastructure - highspeed networks, high-performance computing, 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.

CONTENTS

Cover: Visualization created by Michal Brylinski, assistant professor of LSU's Department of Biological Sciences and the CCT, lead of the Computational Systems Biology Group. Image: A conformational ensemble of blasticidin-S deaminase, an important enzyme in cellular metabolism and a target for antibacterial drugs. Using high-performance computing technologies, structural models can now be routinely constructed from genomic data for hundreds of thousands of proteins using template-based modeling approaches, such as those recently developed by Computational Systems Biology Group @ LSU eThread algorithm.

MESSAGE FROM THE DIRECTOR:

Components provides an avenue through which CCT can highlight the past year's accomplishments of one of LSU's most vibrant and publicly visible research centers. The articles in this volume illustrate the diversity of research and creative projects undertaken by our faculty, staff, and students; how, as a research center, we contribute to LSU's educational mission; how we have helped enhance LSU's cyberinfrastructure in support of computational research across the campus; and ways in which our contributions to the economic development efforts of Louisiana are growing.

As has become routine – and not at all unexpected, given the environment at CCT, which nurtures success – some faculty and staff have left the CCT for positions elsewhere, while others with very promising careers have joined our ranks. Of special note is Stephen Beck's decision to take on the directorship of LSU's prestigious School of Music, effective July 2012. While Steve will retain a joint appointment with the CCT, his time and efforts will now necessarily be focused elsewhere. We owe Steve tremendous gratitude for the key role he has played in creating the Red Stick International Animation Festival, spearheading the AVATAR initiative, and providing the creative insight that has led to every aspect of the CCT's involvement in digital media – not to mention his past service as interim director of the entire center! We greatly appreciate Brygg Ullmer's willingness to step into Steve's shoes as head of the CCT's Cultural Computing Focus Area, moving forward.

Finally, we bid farewell to Ed Seidel, CCT's Founding Director. Please enjoy the tribute to him, as well as the many articles in *Components* that describe CCT's adventures in 2012.

Joel E. Tohline, Ph.D
Director

Photo taken by: Jim Zietz, LSU Office of Communications & University Relations

TRIBUTE TO ED SEIDEL, CCT FOUNDING DIRECTOR

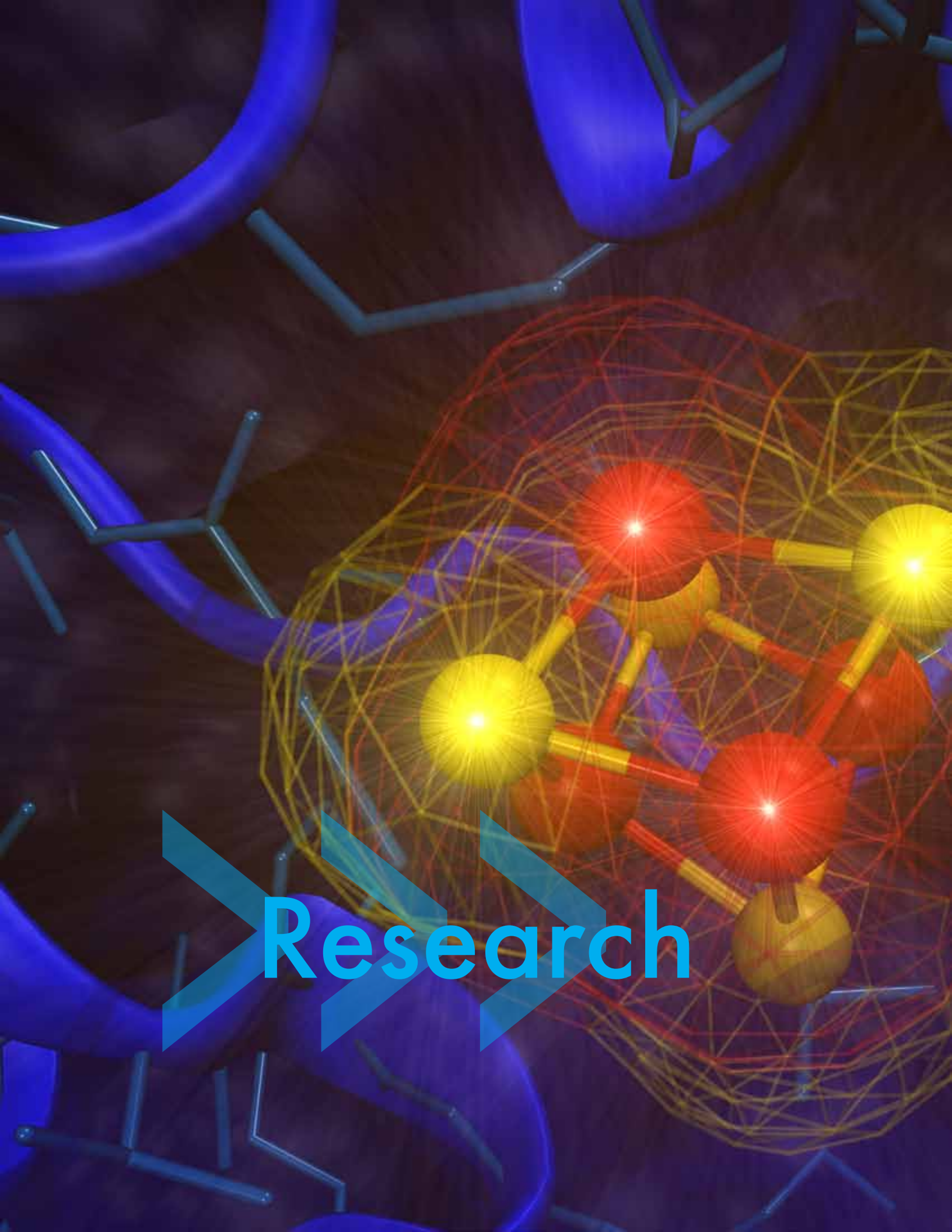
In 1995, the Albert Einstein Institute (AEI) was founded near Potsdam, Germany, as part of the expansion of the Max Planck Society following the reunification of Germany. One year later, AEI's leadership convinced Ed Seidel – a bright, young astrophysicist and computational scientist – to move from the University of Illinois' National Center for Supercomputing Applications (NCSA) to Germany to build a world-class research effort in numerical relativity as part of the AEI's mission to understand the fundamental laws of gravitation. Ed was tremendously successful, focusing a European-wide collaboration of relativists toward the goal of accurately simulating binary black hole mergers and, simultaneously, guiding the early development of a computational and network infrastructure across Europe to support challenging computational research projects.

In 2001, through Governor Mike Foster's leadership, the Louisiana legislature allocated new funding through the Board of Regents to establish and sustain a vigorous research and educational program in the information technology (IT) arena with the expectation that the resulting products of research, including a more technically trained workforce, would help diversify Louisiana's economy. Two years later, LSU convinced Ed Seidel to move from the AEI to Baton Rouge to serve as the founding director of its new Center for Computation & Technology (CCT), which was established as part of Governor Foster's IT initiative. In short order, Ed put the CCT, LSU, and Louisiana on the map! Especially through its resonance with nearby LIGO-Livingston – one of two NSF-funded national observatories designed to detect gravitational radiation from astrophysical sources – the activity of his numerical relativity group immediately enhanced LSU's research profile in the eyes of physicists worldwide. But, more important to Louisiana's statewide higher education community, Ed mapped the vision of a geographically distributed, IT infrastructure that was being implemented across Europe, to Louisiana in the form of the Louisiana Optical Network Initiative (LONI). As we learned through Ed Seidel's leadership, a robust cyberinfrastructure – high-performance computing resources coupled via high-bandwidth networks – not only provides a tangible computational foundation that is essential to research in the modern digital era, but it also greatly facilitates untold virtual collaborative networks among researchers statewide, nationwide, and worldwide.

In 2008, the director of the U.S. National Science Foundation convinced Ed Seidel to take a leave of absence from CCT/LSU and accept an appointment as director of the NSF's Office of CyberInfrastructure: the challenge being to map his vision of a modern research cyberinfrastructure to the nation. In less than two years, Ed was promoted to assistant director of the NSF's largest directorate, Mathematical and Physical Sciences (MPS). It is too early to faithfully measure the long-term impact that Ed's scientific and administrative leadership at NSF has had on the nation. But if it is anything like the impact he had on Europe while stationed at the AEI, or that he had on Louisiana while leading the CCT, the country's research community will be moving forward with a new collaborative vitality.

At the end of summer, 2012, Ed Seidel completed his four-year term of service at the NSF and notified us of his intention to resign from LSU to accept yet another challenge. He has been invited by the Russian government to accept the position of vice president for Research and Innovation at the new Skolkovo Institute for Science and Technology that is being built outside of Moscow. We trust that Ed's decision to explore this new frontier – which mixes promisingly fertile ground in which to plant his transformative ideas with an unfamiliar cultural environment and uncertain political stability – has been buoyed by the success that he (and we!) enjoyed while he was in Louisiana, serving as CCT director.

Thanks, Ed! We wish you all the best.


Research

COMPUTATIONAL SYSTEMS BIOLOGY GROUP FOCUSES ON LARGE-SCALE MODELING

Computational Systems Biology aims to develop and apply efficient algorithms to address critical scientific questions through computer simulations and theoretical modeling. The system-wide level modeling is particularly relevant in modern biological sciences, where 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.

In less than a year at LSU, Michal Brylinski has forged an impressive number of collaborative projects with other computational scientists as well as experimentalists in various departments across LSU. One of the newest faculty members in the Department of Biological Sciences and CCT, Brylinski has formed the Computational Systems Biology Group with a vision to "design and develop novel tools for modeling and analysis of biological networks using computational systems biology."

"What I am really interested in is very large-scale modeling," said Brylinski. "For example, you have a protein of interest and want to know what is its molecular function, does it bind to other proteins, or is it a potential drug target that could be linked to some disease. Studying this protein in isolation is quite problematic, because it is an integral component of an environment where it can interact with tens of other proteins that could modify its function. That is why the research becomes so complicated. It's not enough to study an interesting protein in isolation; you need to put it in a context of a living cell. So you go from the modeling of one protein to the modeling of many or even all proteins in the cell—it changes everything. This is systems level modeling, which is very, very difficult not only in terms of the development of tools that can handle the massive size of the system, but also in the substantial computational power needed to process the data. But the benefit is that some of the properties of the system cannot be captured by studying individual molecules without the cellular environment. You need to put them in the framework of a real biological system. So this is what ideally we want to do—to study systems."

Image (left): Iron-sulfur cluster bound to methyltransferase N. The identification of all iron-sulfur binding proteins across the entire genome of E. coli is the major goal of a multidisciplinary project by researchers from the LSU Department of Biological Sciences and CCT, who combine advanced molecular biology techniques with cutting-edge computational modeling to challenge systems-level biological problems. Credit: Michal Brylinski, assistant professor of LSU's Department of Biological Sciences and CCT.

Modeling biological systems takes a tremendous amount of computational power, and Brylinski uses Queen Bee and other high performance computers in the LONI system and is looking forward to using the new Tezpur replacement, SuperMike II.

"Not only has there been a huge change in recent years in terms of computing power," said Brylinski, "but also in the development of new technologies. GPU computing right now is getting very popular, and that could be very useful for scientific computing. I think the future of scientific computing in many disciplines is system level modeling, and computational biology is a good example of that. In computational biology we very often use a very diverse collection of algorithms that can differ from each other in terms of the required memory, CPU time, IO operations, and network bandwidth.

"So, for example, some algorithms require huge amounts of memory, almost like bioinformatics tools, whereas some algorithms require very tiny amounts of memory but very fast processors and as many as possible. Some algorithms can be developed in a very efficient, parallel manner, which is ideal for GPU computing. We need a heterogeneous platform to run this collection of different algorithms efficiently, so if we build a cluster with some nodes equipped with a large memory, some with very fast CPUs, and add a GPU component, then we can run all those algorithms in a very efficient way. Right now those very heterogeneous platforms are becoming available, so that changes everything. It's both easier and more difficult to use them—because those systems are more complicated, it takes more effort and skills to set everything up, but then you can run it faster, longer, and you can handle much bigger systems."

Part of Brylinski's vision for the Computational Systems

Biology Group is to gradually make tools the group develops available on-line. The goal is for the user to be able to perform most of the calculations directly from the group's Web site.

"I have five or six tools hidden that we are still developing," said Brylinski. "In the next few months, most of them will be available on-line through user-friendly scientific gateways. So you will just submit a job, and you don't really care what happens to your job as long as the results are useful. That is why I collaborate with so many people in computer science and in CCT, because if those Web services become very popular, then we will need some substantial computational power to process the calculations. Right now I have a local multi-core machine, which is set up in CCT, and CCT IT people are helping with that, a lot. Ideally I would like to move most of the calculations to national cyberinfrastructure like NSF's XSEDE, or perhaps LONI systems.

"All of the tools are available for free to the academic community and nonprofit organizations. Also, you can register yourself as a private user. And you can use whatever you want—I don't ask any questions. The only thing that I will ask for is some form of acknowledgement. So if someone uses these Web services and then he or she publishes a paper, I would appreciate a citation. With commercial entities, I will probably come up with a license, initially for a very small amount of money, mostly symbolic, so they can try those methods, test them, and if something works, they can purchase a regular license. So companies, mostly pharma and biotech, will be able to use the tools at very reasonable costs."

Collaborations

"Being a part of CCT makes initiating collaborations much, much easier," said Brylinski, "because we have contact during meetings, seminars, and after seminars, in the hallways or the kitchen, and we just are talking, and then it turns out we have so much in common that we didn't even realize. Then we initially start informal collaborations on different projects, and at some point perhaps we will have some results that could lead to a couple of publications, and then a formal proposal, submitted jointly to a funding agency, most likely NSF or NIH. So that's why CCT is a really good place to foster those kind of collaborations; all those people who have common interests are in one place, running into each other, so naturally those collaborations just pop up.

"Right now I have several ongoing collaborative projects with the members of CCT. For example, Joohyun Kim, Nayong Kim, Shantenu Jha, and I are working on setting up a collection of scientific gateways to make available some of the tools that we are developing in our group to the academic community through the XSEDE project."

Michal Brylinski considers creating the visualizations of his research as a kind of side hobby—a hobby that has resulted in his images appearing on the cover of three prestigious journals (*Proteins*, *JCIM*, and *PCCP*).

"Right now there are so many tools that you can use to make really cool visualizations of molecular systems, and many of those tools are open source, so you can just download them and play with them. Those results can be embellished with a little more advanced rendering software.

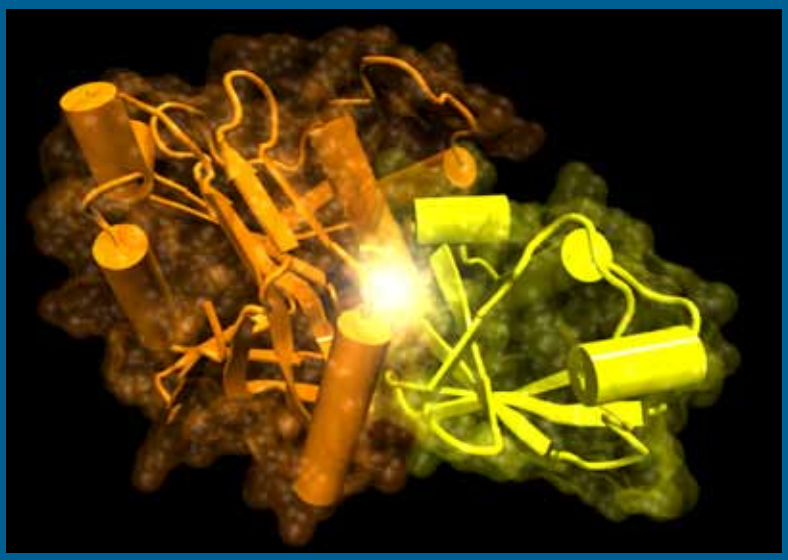
"For bigger projects, I try to create an image that will illustrate what the project is about. Many of our projects involve drug design and discovery, which is very nice thing to illustrate. Most drugs bind to their targets, typically proteins, so you have a macromolecule, very sophisticated, and then you have a drug compound that binds somewhere. This biologically relevant association is a very nice thing to visualize. You can present the protein as a surface, and then include a representation of the drug that binds.

"Another type is iron-sulphur proteins, which are more like organic clusters. They also bind to proteins, so you can also present the protein with the binding site, and the cluster binds somewhere, and then you can tweak the lights, make some shadows, and add some very nice, bright colors.

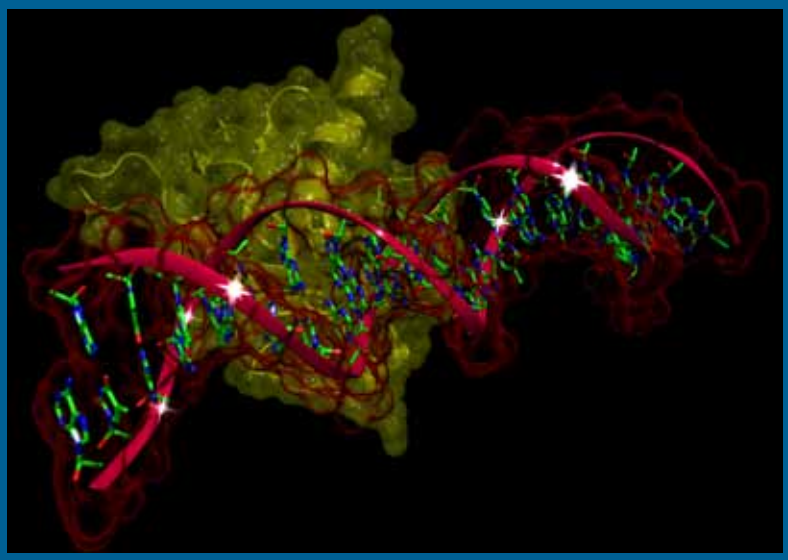
"Protein/protein interactions can also be visualized in a very nice way. All the visualization tools that were developed for drugs, for example, or for some other networks, can be used to visualize biological networks too.

"I also have been collaborating with some CCT professionals in visualization effects."

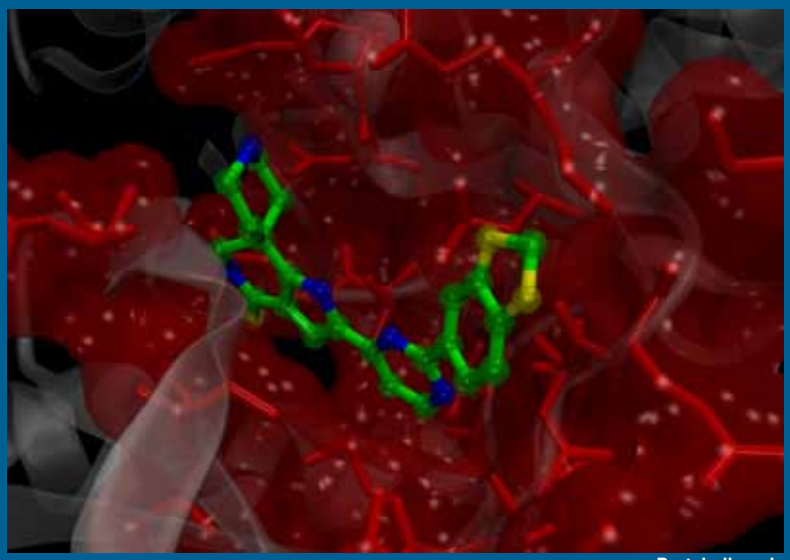
For now, Brylinski is doing only static images, stills, but there are also tools for molecular movies, and later he might try expanding his side hobby in that direction.



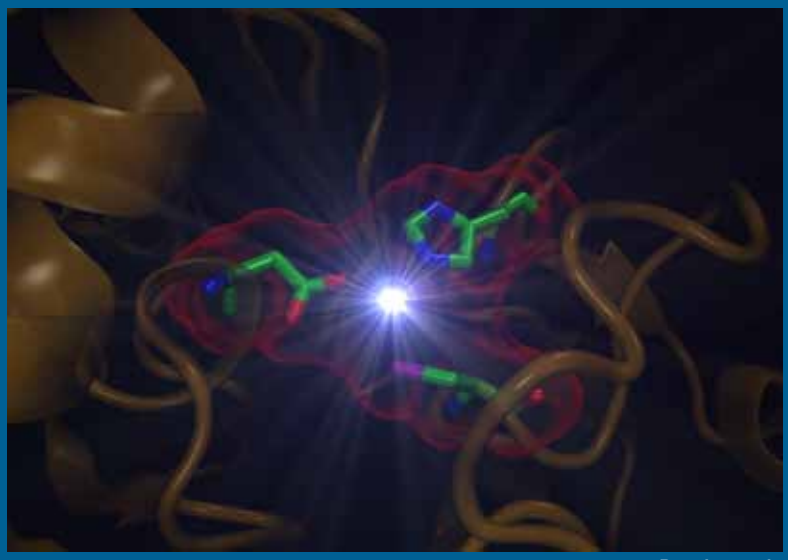
Protein-protein



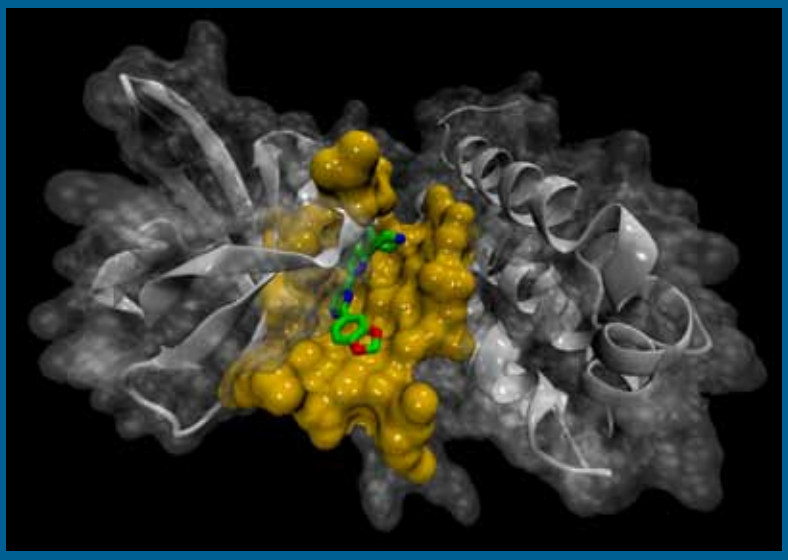
Protein-DNA



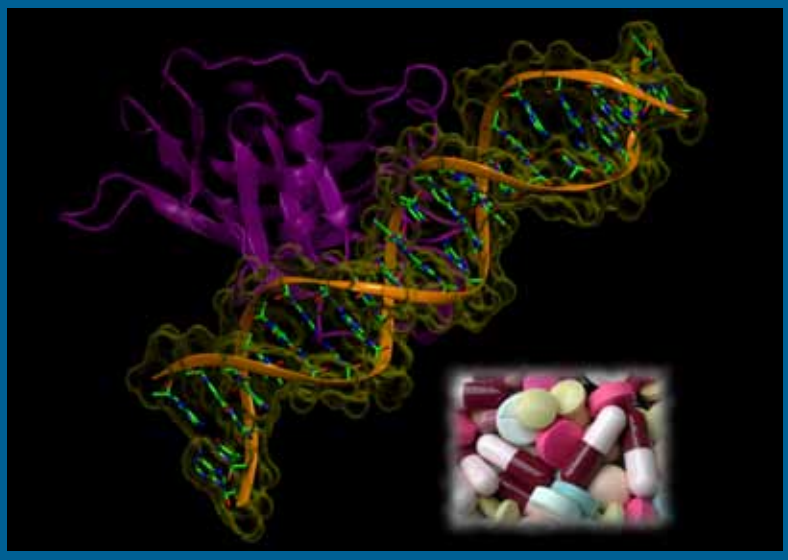
Protein-ligand



Protein-metal



Functional Genomics



Pharmacogenomics

All images created by Michal Brylinski
Brylinski.cct.lsu.edu

"I also collaborate with Jay Park, who is in the Division of Computer Science and CCT. We are focusing on using distributed clusters and the Apache Hadoop technology for modeling proteins on a really large scale. We want a user to be able to just submit his or her jobs for large scale modeling in a way that is as simple as possible, and totally transparent, so he or she doesn't even realize how powerful the infrastructure is behind the scenes.

"Mark Jarrell, Juana Moreno, Ram Ramanujam, David Koppelman, and I, as well as other people from the LA-SiGMA team, are trying to explore new ways of conformational sampling in material science. This particular project, which is part of the broader computational biomaterial focus of LA-SiGMA, mostly involves ligand docking and has very good applications in drug development and the design of new drug delivery systems. We've found that we have lots of overlap between our research projects. For example, physicists extensively use Monte Carlo techniques to sample conformation space to study the properties of highly correlated materials. And I also sample conformational space but for drug design. The interesting thing is that the techniques we use are almost identical, so right now we are trying to develop a very general framework for Monte Carlo methods that can be used pretty much anywhere – in physics, astrophysics, biology, chemistry—so this is a very, very promising project."

In the chemistry and biology departments, Brylinski also works with experimentalists. "They really appreciate the help from computational groups," Brylinski said. "Right now the problem is there is so much data, and so many directions that the projects could go, that they sometimes cannot select the best way to proceed with the project. If there is someone who can do some modeling and guide the experiment, they are really interested in that, because that will clarify some things, minimize the costs, and ultimately maximize the chance of success. With Huangen Ding in biological sciences, I work on identification of all iron-sulfur binding proteins in the *E. coli* genome. This is a very good example of such a collaborative project, because there are more than 4,000 gene products in this particular genome. Some of those proteins bind iron-sulfur clusters, and some don't. Ding's problem is that he cannot test 4,000-5,000 proteins experimentally. He can probably test a few tens of them, though he doesn't know which experiments to carry out on this particular genome. But I can do some modeling and provide a list that identifies those proteins that most likely bind iron-sulfur clusters; then he can focus on those proteins and confirm that bioactivity.

"Another similar project is with Grover Waldrop from biological sciences. We are working on a new class of antibiotics. We have maybe a handful of compounds with confirmed activity toward a particular enzyme that we are interested in, but there are only a few of the compounds, and they are not perfect. They are not broad enough, so they can kill maybe two or three bacterial species, but not all of them, and not the most virulent. So again, I can use this experimental data to develop some models and procedures to come up with new antibiotics, which would be broad spectrum, so could kill the more virulent bacteria species. There are four or five research groups across LSU campus involved in this effort. This is a very exciting project that actually was abandoned by a pharmaceutical company, because this is not profitable enough for commercial research. But Waldrop was encouraged to pick this project up and carry on in an academic setting. We are less subject to financial constraints than pharmaceutical companies, so we can do something that is less profitable, but it is exciting and it can help a lot of people."

For the spring semester, Brylinski will develop a course in computational biology. "There are very good, strong courses in both computer science and biology, but there are not that many overlapping courses, like computational biology or bioinformatics. That would be something very useful for graduate students, because as undergraduates they can take those individual courses first, like computer science, programming, or scientific computing, and then biology or biochemistry courses. Later in grad school they can take more advanced courses like computational biology that would require both biological and computer science courses and combine those two disciplines. Also, with Jeremy Brown from biological sciences and Brygg Ullmer from computer science and CCT, we plan to launch a monthly undergraduate outreach lecture series at LSU, which is intended to expose students from biology, mathematics, and computer science to current and exciting research in bioinformatics and computational biology."

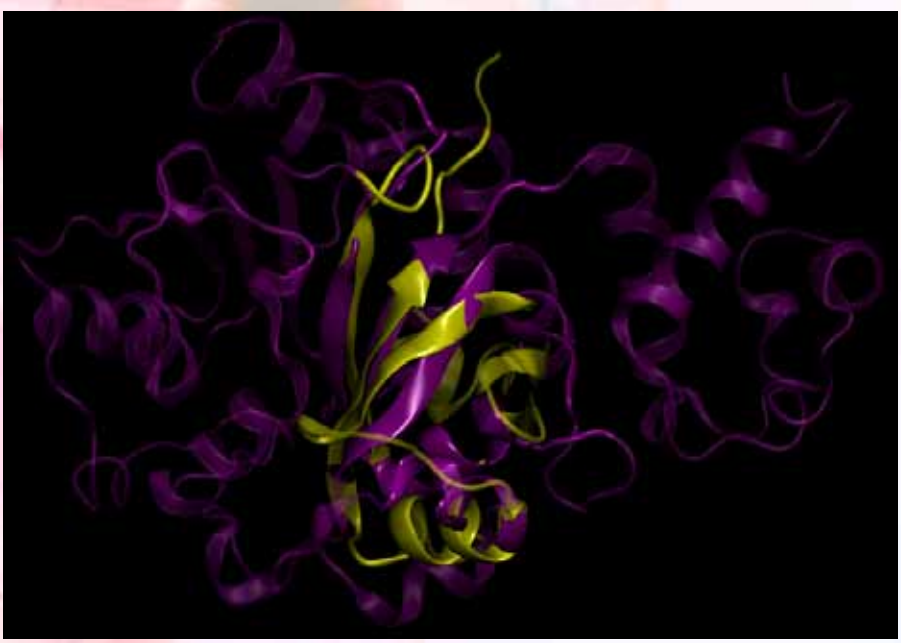
In discussing the Computational Systems Biology Group, Brylinski said, "Ideally I would like to talk about a larger group of people. Right now I have one postdoc and one graduate student, both from the biology department, one undergraduate student from chemistry, and two undergraduate students from physics. Another graduate student will be coming in the spring. So, including me, that's seven people—a small group right now. I will do my best to keep the collaborations I've discussed going. Once we start getting some interesting results and publications, then I will expand the Web site to include the bigger picture, and the other research groups that we collaborate with. We will include all the descriptions of the research projects, the preliminary results, sources of funding, and new tools, and continually expand this Web resource."

Another way Brylinski would like to expand the Computational Systems Biology Group is by attracting more students, both graduate and undergraduate. "Graduate students find me because they are already interested in this specific type of research." His graduate students and a postdoc have backgrounds in computational biology, bioinformatics, computer

science, and basic medical sciences.

"It is very different for undergraduate students," said Brylinski, "because they think all of this is cool stuff. Typically, they don't really have a solid background, but they are well-motivated, and they want to do something that is relevant, important, and also fun to do, and this is a good example of something like that. It's lots of fun doing this—lots of frustration, too, but rewarding, because this is important, and it can make a significant difference in the field. So I just give them the opportunity to try it. Many of them like it, because it is so diverse they can go in many different directions. They can focus on the computer science aspect and work on high performance computing, GPU computing, grid and cloud computing, all those advanced technologies that are out there. Or they can focus on specific biological problems: drug design, protein structure and function modeling, or neuroscience, for instance. There are many, many directions that they can go."

"I'm constantly looking for good, motivated students, so if anyone is interested, please get in touch!"



ORAU
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LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

NVIDIA

LSU
LOUISIANA STATE UNIVERSITY

Exploring Origins of the Universe

Parampreet Singh, assistant professor in the LSU Department of Physics & Astronomy, and Peter Diener, assistant research professor in the LSU Center for Computation & Technology and the LSU Department of Physics & Astronomy, recently received a $250,000 grant for a potentially breakthrough proposal hoping to answer questions about the earliest state of the universe.

The grant, funded by the John Templeton Foundation, awarded more than $4 million in research grants to 20 scientists worldwide.

More than 300 proposals were submitted to address questions that have the potential to expand the boundaries and deepen the foundation of scientific inquiry.

Singh and Diener chose to focus their proposal on the fundamental question regarding the origin of the universe, which has so far eluded scientists.

It is generally thought that Einstein's theory of general relativity, which is successful in describing the universe when gravitational force is weak, predicts that the universe began with a big bang — an event where all the matter and energy of the universe was concentrated at one point. Unfortunately, Einstein's theory itself breaks down at this point, called a singularity, and cannot predict the earliest state of the universe.

"The goal is to discover a new theory which avoids the problem of big bang singularity, and also captures all the success of Einstein's theory when gravity is weak," said Singh.

One such theory is loop quantum gravity. LSU's theoretical gravity group at the Department of Physics & Astronomy is one of the major centers in the world for research on this subject.

Singh and Diener will harness the power of high performance computers at LSU and other centers in the U.S. to develop sophisticated algorithms to fully understand the new physics near the singularities in cosmos and black holes.

Singh is an expert on quantum cosmology and has made several important contributions to the field, including in the development of big bounce paradigm in loop quantum gravity, which theorizes that our expanding universe did not start from a big bang, but there existed a contracting branch of our universe to which it bounces.

Diener is an expert on relativistic astrophysics and one of the key maintainers of the Einstein Toolkit. He is involved in the development of various supercomputing applications to understand various aspects of gravitational force including the dynamics of black holes.

LSU CCT PART OF NATIONAL COLLABORATION TO ADVANCE DOE COMPUTING

CCT will play a major role in the recently awarded U.S. Department of Energy grant to advance extreme-scale computing. The overall proposal, led by Ron Brightwell of Sandia National Laboratories, was awarded $7.05 million. Other research partners include Oak Ridge National Laboratory, Indiana University, University of Houston, University of Oregon, University of North Carolina at Chapel Hill, and the University of Delaware.

The research and software prototype development project was delivered to the DOE Office of Science through its 2012 X-Stack Program of Programming Challenges, Runtime Systems, and Tools. The project will produce a revolutionary software system for extreme-scale computing for both Exascale and strong-scaled problems.

Titled XPRESS, meaning eXascale PRogramming Environment and System Software, it will enable Exascale performance capability for DOE applications, both current and future; develop and deliver a practical computing system software X-stack, "OpenX", for future practical DOE Exascale computing systems; and provide programming methods, environments, languages, and tools for effective means of expressing application and system software for portable Exascale system execution.

CCT's STE||AR group, led by Hartmut Kaiser, senior scientist of the CCT and adjunct professor of the LSU Division of Computer Science, will bring an extensive skill set and manpower to the project.

"Our 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," said Hartmut Kaiser, lead of the STE||AR group. "The highly modular structure of HPX guarantees a smooth migration path from today's systems towards future architectures, which provides a stable implementation platform for application developers over the next years. We are very proud to enable scientists to achieve results today that they couldn't achieve purely using conventional programming models."

HPDC TOP PAPER AWARD RECEIVED

LSU's Gabrielle Allen, Werner Benger, Andrew Merzky, and Ed Seidel are co-authors of a research paper designated by the International ACM Symposium on High-Performance Parallel and Distributed Computing (HPDC) as one of the top 20 papers in the past 20 years of publications.

HPDC is the premier computer science conference for presenting new research related to high-performance parallel and distributed systems used in science and industry. Since its inception, HPDC has been at the center of new systems discoveries such as clusters, grids, clouds, and parallel and multicore computers.

Published in 2000, *"The Cactus Code: A Problem Solving Environment for the Grid"* explained how the intensive computing requirements of physics applications using the Cactus Code encourage distributed and metacomputing, described the development of and experiments performed with Cactus, and detailed how its design made it an ideal application test bed for Grid computing.

Originating in the academic research community, Cactus has been developed and used over many years by a large, international collaborations of physicists and computational scientists. Specifically, Cactus is an open-source problem-solving environment designed for scientists and engineers. Its modular structure facilitates parallel computing across different architectures and collaborative code development among different groups.

The Cactus group at CCT continues to innovate in software that advances both physics and computer science, and in particular leads the development of the Einstein Toolkit to provide a cutting edge toolkit for relativistic astrophysics that has been adopted by some 60 groups around the world.

Members of the HPDC community at large nominated papers for the award, and a special committee narrowed the list to the best 20. A special edition containing the 20 papers was distributed at HPDC's 2012 meeting in Deflt, The Netherlands.

G. Allen, W. Benger, T. Goodale, H.C. Hege, G. Lanfermann, A. Merzky, T. Radke, E. Seidel, and J. Shalf, *The Cactus Code: "A Problem Solving Environment for the Grid,"* The Ninth International Symposium on High-Performance Distributed Computing, 2000. Proceedings, IEEE, 2000, pp. 253–260.

LSU RECEIVES $1 MILLION TO EXPLORE NEW ENERGY SOURCE FROM RESERVOIR HEAT EXTRACTION

A group of LSU researchers is conducting innovative research to harvest heat from geothermal reservoirs to generate electricity. The proposed method couples forced convection through long, near-horizontal wellbores with free convection arising from natural geothermal gradients.

Christopher White, associate professor, and Mayank Tyagi, assistant professor, both of the LSU Craft and Hawkins Department of Petroleum Engineering and the CCT, along with other LSU researchers, were awarded a grant for $997,333 from the U.S. Department of Energy for the project "Zero Mass Withdrawal, Engineered Convection, and Wellbore Energy Conversion."

Compared to conventional geothermal development strategies, engineered convection improves thermal recovery efficiency and delays thermal breakthrough of heat-depleted geofluid at the heat extraction point. Computer simulations indicate that the engineered convection strategy could be effective for the saline aquifer temperatures, thicknesses, extents, permeabilities, and dips that are common in the U.S. Gulf Coast region.

"Low-cost, environmentally benign geothermal energy could boost the economy of the region, especially in socioeconomically disadvantaged areas and remote areas with poor electric power transmission and transportation infrastructure, such as the coastal wetlands," said White, principal investigator of this project.

The engineered convection strategy could provide robust, modular power with individual wells contributing hundreds of kilowatts up to megawatts in net electric power, potentially adding up to a regional capacity of tens of gigawatts by the year 2050.

"Engineered convection geothermal systems could be made robust with respect to floods and storms by placing some of the energy conversion components in the wellbore, providing valuable emergency and post-hurricane distributed power. In-wellbore generation could also reduce the surface facilities footprint, reducing noise and potentially reducing water requirements," said White.

Also participating in the project are Arash Dahi Taleghani, Richard Hughes, and Mileva Radonjic, LSU Craft and Hawkins Department of Petroleum Engineering; Jeffrey Hanor, LSU Department of Geology & Geophysics; Chacko John, Louisiana Geologic Survey; Mark Kaiser, LSU Center for Energy Studies; Fahui Wang, LSU Department of Geography & Anthropology; and Blaise Bourdin, LSU Department of Mathematics and CCT.

Software Infrastructure for Tensor Computations

CCT Professor Ram Ramanujam and Associate Professor Gerald Baumgartner, both of the LSU School of Electrical Engineering & Computer Science, are working on a newly-funded NSF project to build an advanced software infrastructure for continuing research on compiler optimizations for tensor computations. Motivated by the successes of the model-driven search-based optimization approach of NSF, DOE, and Army funded Tensor Contraction Engine (TCE) and the polyhedral model-based transformations (PLUTO) projects, this project will develop an optimization infrastructure that combines the key aspects of the TCE and the polyhedral models and provides the flexibility to continue research on optimizing and automatically parallelizing tensor computations for parallel and/or distributed computations for any machine architecture, including multicores and accelerators such as GPUs.

"This novel optimization framework has potential for high payoffs in enabling future research and eventually in generating high-performance code for an important class of quantum chemistry codes and other tensor computations," said Ramanujam. "After further research, it will become a valuable tool for reducing the time to develop high-performance applications in several areas of science and engineering."

Theda Daniels-Race, Ph.D.

THEDA DANIELS-RACE RESEARCHES NON-TRADITIONAL ENERGY

After the BP oil spill and with economic and political demands to lessen dependence on fossil fuels, Louisiana is actively supporting research toward the development of alternative energy.

Theda Daniels-Race, associate professor of the LSU Division of Electrical & Computer Engineering and the CCT, received $147,194 from the Louisiana Board of Regents to discover how combinations of new hybrid materials can be used in non-traditional means of energy production, transmission, and storage. Daniels-Race's proposal titled "Nanoscale Electronic Characterization of Hybrid Electronic Materials" was funded for a three-year period.

"As the words alternative energy can be applied to a broad range of engineering technologies, in this work we will investigate the basic science behind these potential applications from a very fundamental electronic materials perspective—that is, at the molecular/nanoparticle level. In this way, we not only have the opportunity to observe new science, but we will be able to learn about, and therefore exploit, the fundamental physicochemical properties needed to engineer hybrid materials and their functions in alternative energy processes," said Daniels-Race.

A new form of hybrid electronic materials (HEMs), known as GUMBOS, or a Group of Uniform Materials Based on Organic Salts, will be investigated. GUMBOS were recently discovered by LSU Vice Chancellor Isiah M. Warner of the Office of Strategic Initiatives, Boyd Professor and Philip W. West Professor of Analytical & Environmental Chemistry. They represent a first in that they are a new nanomaterial composed of ionic liquid species in the frozen state.

"What is different about GUMBOS," said Daniels-Race, "is that, unlike traditional ionic liquids that have melting points less than 100 degrees Celsius, GUMBOS can be synthesized to exist in the solid-state as nanoparticles in the 25 to 250 degrees Celsius range. As designer nanoparticles, their properties can be tailored to meet a host of applications in areas ranging from energy to biomedical functions to environmental uses. GUMBOS provide the prospect of utilizing new science with the objective of addressing fundamental alternative energy needs of efficiency, lower production costs, and materials-to-device engineering and development."

Daniels-Race will work with Warner and his group, who will provide the GUMBOS needed for the research.

"We believe that in this study of HEMs for alternative energy applications, we combine the discovery of new materials with exciting engineering developments in an area of urgent national interest," said Daniels-Race. "As conventional and highly developed electronic materials, such as silicon, reach their predictable limits, and the nation's focus upon alternative means of energy production increases, this investigation stands well-poised to meet the academic and practical demands for new discoveries."

From left to right are as follows: Theda Daniels-Race, PhD; Hao Wang; Madhavi Divakar Rajathadripura; Giovoni King; Kalyan Kankamedala; and Anirban Sarkar.

FIRST-EVER SYMPOSIUM ON LAPTOP ENSEMBLES AND ORCHESTRAS

symposium on laptop ensembles & orchestras

The first-ever Symposium on Laptop Ensembles and Orchestras, or SLEO, an international workshop on music performance using laptop computers and mobile devices such as smartphones and iPads, was held April 15-17, 2012, at LSU. "The goal of SLEO was to help establish a set of best practices for laptop ensembles, presentation of cutting edge technologies – like the hemispherical speakers that are used by both Sideband and the Laptop Orchestra of Louisiana, or LOLs– and workshops to help aspiring electronic musicians begin their own laptop or mobile ensembles," said Stephen David Beck, director of the LSU School of Music and of the LSU-based LOLs. "Never before has such a group of leading researchers convened to discuss the future of laptop-generated music."

International submissions were accepted for workshops, papers, panel discussions, posters, demonstrations, and music composition for laptop ensembles and orchestras, or LEOs. Topics included best practices in composition; rehearsal; performance; techniques used in composing for LEOs; software and network management; history and aesthetic theory of LEOs; teaching and pedagogical strategies; hardware including audio, interface, computers, and loudspeakers; software environments and frameworks; and composers' perspectives on their own musical compositions.

Some of the world's leading ensembles performed at SLEO, including the Mobile Performance Group of Stetson University, Sideband of Princeton University, the Linux Laptop Orchestra from Virginia Tech University, the European Bridges Ensemble from Germany, and LSU's LOLs.

The symposium was sponsored by CCT, the LSU Arts, Visualization, Advanced Technologies and Research (AVATAR) initiative in digital media, and the LSU School of Music, with cooperation from Princeton University and Stetson University.

STE||AR

STE||AR's activities are centered around the ParalleX execution model and its implementation in their experimental runtime system HPX (High Performance ParalleX). HPX is used for a broad range of scientific applications, helping scientists and developers to write code that scales better and shows better performance compared to more conventional programming models such as MPI.

HPX RELEASED

The first open-source runtime system implementation of the ParalleX execution model, called HPX, or High Performance ParalleX, is now available. It is a general purpose C++ runtime system for a parallel and distributed applications at any scale.

HPX is being provided to the open community for experimentation and application to achieve high efficiency and scalability for dynamic adaptive and irregular computational problems. HPX is a library of C++ functions that supports a set of critical mechanisms for dynamic adaptive resource management and lightweight task scheduling within the context of a global address space. It is solidly based on many years of experience in writing highly parallel applications for HPC systems.

HPX is designed to enable developers to exploit the full processing power of many-core systems with an unprecedented degree of parallelism. The highly modular structure of HPX guarantees a smooth migration path from today's systems toward future architectures, which provides a stable implementation platform for application developers over the coming years.

HPX development has been sponsored, in part, by the National Security Agency, National Science Foundation, DARPA (Defense Advanced Research Projects Agency), and Microsoft, as well as by the LSU CCT.

STAR: ASTROPHYSICS RESEARCH

STAR has launched!….Scalable Toolkit for Transformative Astrophysics Research creates a new model of computation that radically benefits applications that support studies of the evolution and merger of close binary star systems. When scaled to reflect physically meaningful domain sizes and resolutions, the model could potentially transform the understanding of stellar evolution.

"The impact of this research isn't limited only to the advancement of astrophysics, computer science, and engineering, but also significantly affects the fields of computational sciences as a whole by enhancing the understanding and capability of efficient realization of scalable computing of any size. This capability extends beyond the conventional means and practices in that it targets the difficult strong scaling problem in addition to supporting the traditional weak scaling regime so prevalently employed on the largest supercomputing platforms of today," said Hartmut Kaiser, lead of the CCT STE||AR group and adjunct associate research professor of LSU's School of Electrical Engineering & Computer Science.

Funding is provided by the National Science Foundation's new INSPIRE grant program. INSPIRE, which stands for Integrated NSF Support Promoting Interdisciplinary Research and Education, was established to address some of the most complicated and pressing scientific problems that lie at the intersections of traditional disciplines.

Systems Technology, Emergent Parallelism, and Algorithm Research Group

STE||AR, a CCT research group focusing on system software solutions and scientific application development for hybrid and many-core hardware architectures, leads real-world applications.

⇢ **http://stellar.cct.lsu.edu/**

GRAPH COMPUTATIONS MADE EASIER!

Several universities across the United States have come together to develop a new environment for graph-based applications, solving a critical need for researchers in science, engineering, and informatics.

Led by Indiana University, the "PXGL: Cyberinfrastructure for Scalable Graph Execution" project will include a parallel programming model for graph computations, a corresponding execution platform, a graph-optimized soft-core architecture, and a graph library. LSU is among the collaborators for the project, led by Hartmut Kaiser, team lead of the CCT STE||AR group. Others include members from New Mexico State University and Sandia National Laboratories.

The importance, applications, and scale of data-centric computing have grown dramatically. The computational resource requirements for graph-based computations for large-scale applications are just as vast as for traditional compute-intensive science, thus there is a pressing need to expand the scope of high-performance computing to include graph-based computations. Problems plague graphic computations, however, because they are often completely data driven, have poor locality, and result in fine-grained data accesses, or a high ratio of data accesses to computation.

PXGL (ParalleX Graphic Library) is an integrated hardware and software framework for solving large-scale graph problems, enabling and facilitating efficient execution of dynamic graph applications on current terascale and petascale systems, as well as future exascale systems. PXGL will enable and fundamentally improve scalability and user productivity for graph-based applications.

In addition, the project will create an experimental processor core called ELVIS (Edge-Linked Vertices Information System) to provide a new compute model for solving graph problems. ELVIS will serve as a vehicle to test the hypothesized requirements of a computer system to efficiently perform graph computation. The teams hope the combination of a non-coherent global address space, multithreading, fine-grained synchronization, and lightweight active messages will lead to the creation of substantially simpler processor architectures capable of supporting graph-based information processing. ELVIS is a unique opportunity to rethink computing as the traditional building-blocks for computer architectures—heavyweight threads, cache coherency, and hardware speculation—are unsuited to graph-based analysis.

The four institutions the PXGL project brings together all have significant experience in particular areas related to large-scale graph processing, and together provide the unique set of capabilities necessary to successfully develop the entire hardware and software system. Development of the parallel graph components of this work will be primarily conducted by the Indiana University team. LSU will be in charge primarily of the HPX runtime development. New Mexico State University and Sandia National Laboratory will be the co-architects of the processor and memory hardware systems. The teams will work closely together to integrate their effort into PXGL and to collaborate with application developers

This project is funded by the National Science Foundation.

JUNIOR FACULTY ACHIEVEMENTS

MICHAL BRYLINSKI

Oak Ridge Associated Universities, a consortium of doctoral-granting academic institutions, awarded its Ralph E. Powe Junior Faculty Enhancement Award to Assistant Professor Michal Brylinski of LSU's Department of Biological Sciences and the CCT. The Powe Award recognizes exceptional academic work by university junior faculty within several disciplines: engineering or applied science; life sciences; mathematics and computer science; physical sciences; and policy, management, or education.

Brylinski conducts research in the area of computational biology at LSU. His group is interested in the development of novel tools for the modeling and analysis of biological networks using computational systems biology, with applications in emerging areas of contemporary life sciences such as the study of multiple drug-drug interactions and the development of more selective and safer therapeutics.

XIN LI

Xin Li, assistant professor of the LSU Division of Electrical & Computer Engineering and the CCT, was one of 24 recipients of the IBM Faculty Award in the fourth quarter of 2011. Li received the maximum award amount of $40,000.

The IBM Faculty Award is a highly competitive international program that intends to foster collaboration between researchers at leading universities worldwide and those in IBM research, development, and service organizations.

Li received the award based on his research of geometric information analysis and processing and its application to computational medicine. Li's research group is currently developing a computational framework to model the respiratory motion of a tumor and surrounding organs, which could guide the automatic offline planning and intelligent online management of lung radiotherapy.

GEORGIOS VERONIS

With a recent grant from the NSF totaling $240,000, Georgios Veronis, assistant professor of the LSU Division of Electrical & Computer Engineering and the CCT, is exploring nanoscale plasmonic structures and devices for enhancement of nonlinear optical effects, all-optical absorption switches, ultra-compact sensors, and plasmon-enhanced thin-film photovoltaic solar cells. The project is called "Plasmonic Devices for Controlling Light at the Nanoscale."

The results of the project may lead to new opportunities for device applications, which will represent important breakthroughs in integrated optics, optical information processing, and renewable energy sources.

SHAWN WALKER

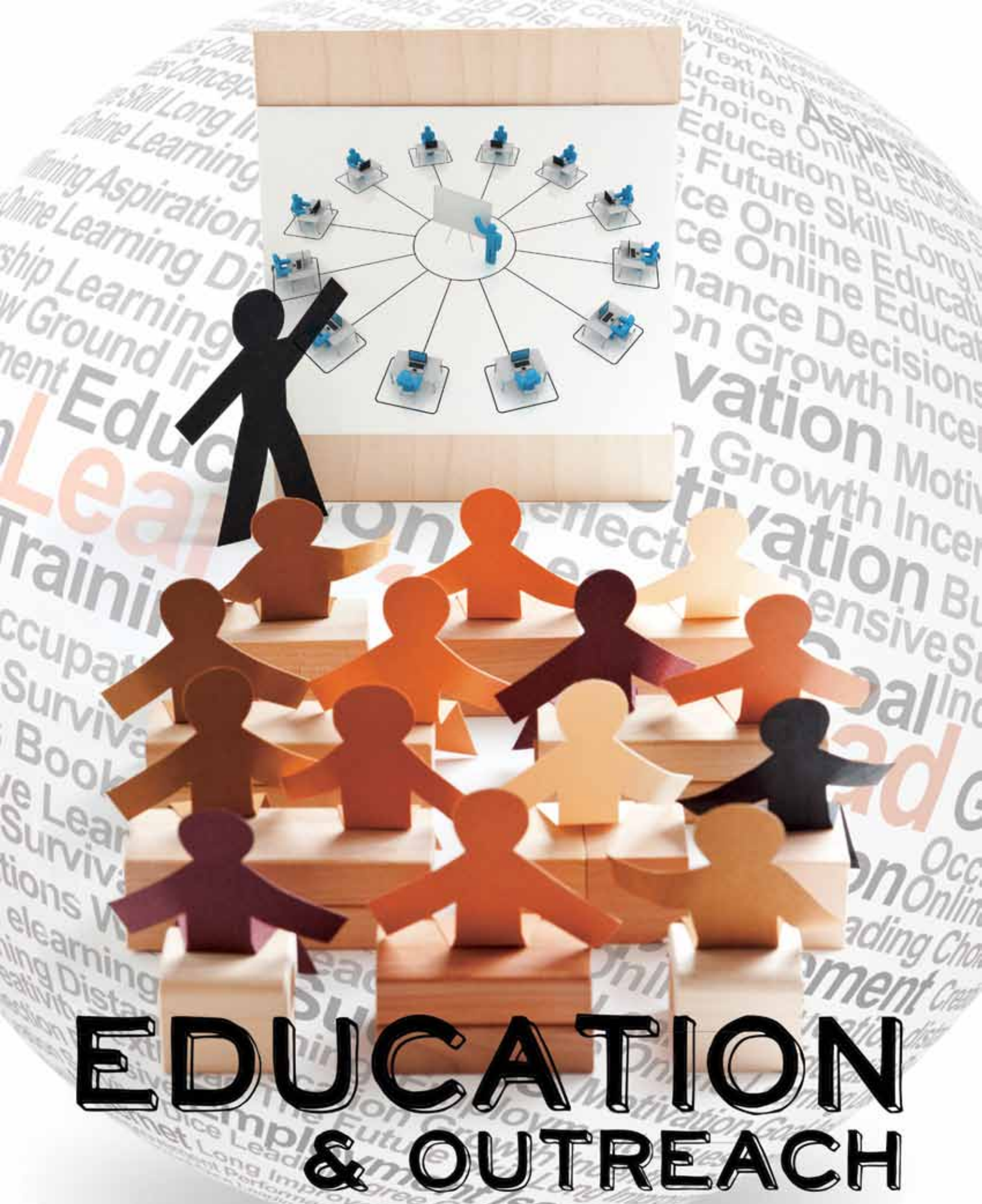
Exploring the math behind the movement of fluids and other objects that have complex moving boundaries has garnered National Science Foundation funding for Shawn Walker, assistant professor of the LSU Department of Mathematics and the CCT.

The project "Numerical Methods for Free Boundary Problems: Two-Phase Flows and Contact Line Dynamics," received $90,657. Results of the research will improve the control and design of industrial processes by bringing together cutting-edge modeling, analysis tools, and computational free boundary techniques in key application areas to expand and investigate the mathematical framework that models these time-dependent, domain-deforming problems.

XIAOLIANG WAN

Xiaoliang Wan, LSU assistant professor of the LSU Department of Mathematics and the CCT, received a $100, 211 award from the National Science Foundation to study the effect of Wick-type stochastic modeling and define possible new applications.

The project plan is to develop new algorithms to quantify the uncertainty in stochastic mathematical models of complex physical systems. Stochastic modeling is used, for instance, to develop simulations to support petroleum reservoir management, probabilistic financial decision making, and probabilistic weather forecasts.


EDUCATION
& OUTREACH

VIRTUAL CLASSROOMS GAIN MOMENTUM

THE LA-SIGMA PROJECT GOES THE DISTANCE

The CCT has been a pioneer in the development of innovative distance learning courses. Since 2008, twenty-three video-conference courses have been taught to support computational materials science at LSU. These synchronous learning courses are an essential component of the Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA) project, funded by the National Science Foundation and the Louisiana Board of Regents. Upper level undergraduate and graduate courses in computational materials science are shared via video-conferencing between Louisiana universities and our international partners. This moves us towards LA-SiGMA's main goal of developing the critical mass needed to be internationally competitive in the field of computational materials science, a critical mass which does not exist at any one of the LA-SiGMA institutions alone.

The LA-SiGMA distance learning courses give our students access to advanced graduate courses that they otherwise would not have. These include courses in computational materials science, such as computational many body theory, to specialized courses in GPU programming, or courses in advanced programming methods. These courses are taught by LA-SiGMA faculty throughout the state as well as our international collaborators. For example, this fall internationally renowned computational physicist Matthias Troyer is teaching Programming Techniques for Scientific Simulations, which is open to all LSU graduate students. This course allows our students to learn modern computer language in the context of realistic scientific applications. Students may also take Many Body Theory with Mark Jarrell at LSU or Simulations of Quantum Many Body Systems. The latter course is taught by faculty throughout North America, including LSU faculty, and Europe (ETH Zurich, LMU Munich, ENS Paris, MPI Dresden), each in their own area of expertise. Courses on GPU programming and optimization taught by LSU faculty Ram Ramanujam or David Koppelman, as well as a course in Computational Physics taught by Juana Moreno (LSU) and Karen Tomko (Ohio Supercomputer Center), are also offered regularly.

All 23 video-conference courses have been shared with LA-SiGMA international collaborators in Germany, India, Switzerland and other countries. LA-SiGMA faculty and students participate in courses that are taken by students all over the world, greatly enhancing the profile of LA-SiGMA and LSU. As a result of these courses, many international researchers have developed collaborations with LA-SiGMA research groups.

These efforts are enhanced by modern high-definition (HD) video equipment purchased by LA-SiGMA and the Board of Regents. An HD video node will be installed at each of the LA-SiGMA institutions (Tulane University, Xavier University, University of New Orleans, Southern University and A&M College, Louisian Tech University, and LSU) with a main switching unit at LSU. This will allow the associated faculty to share courses, research seminars, and meetings with high quality video and sound, and automatically rip these meetings into Web downloadable formats, thus enabling asynchronous learning in addition to the current synchronous methods.

The CCT and LA-SiGMA faculty are leading LSU's effort in developing and teaching a wide array of distance learning courses needed to support growing graduate and undergraduate programs in the computational sciences. This program not only allows us to reach more students, but it also allows us to compete effectively for students.

LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

http://lasigma.loni.org

The Alliance pushes the scientific frontiers in computational materials science, and prepares Louisiana researchers to use the next generation of heterogeneous, multicore and hyper-parallel cyberinfrastructure effectively. LA-SiGMA builds statewide interdisciplinary research collaborations involving computational scientists, computer scientists and engineers, applied mathematicians, theorists, and experimentalists. Most significantly, the Alliance builds materials science graduate curricula that are unique in its statewide reach and impact, and is a model for virtual organizations for advanced education and training of graduate students and post-doctoral fellows.

VIDEO GAME DESIGN COURSE TAUGHT VIRTUALLY

A team-structured, project-oriented, technology-centered introductory Video Game Design Course (LSU computer science CSC 4263) takes full advantage of distributed technologies to create a virtual classroom, shared between LSU in Baton Rouge and the University of Illinois at Chicago (UIC). Robert Kooima at LSU and Jason Leigh at UIC collaboratively teach the course, which enrolls up to 30 students at each site.

A rich ambient connection between classrooms is created with several cameras and displays that use facilities installed and managed by CCT. Large projection systems deliver full-duplex high definition video showing the presenters at both ends of the connection. When necessary, a second high definition video channel delivers a PC desktop allowing Powerpoint presentation and software demonstration, but in the vast majority of cases, the primary video channel conveys enough detail that slides and demonstrations are received naturally, with the speaker interacting directly with them. Meanwhile, a multi-channel audio system mixes the sound of both presenters, all students, and game audio from both live demonstrations.

The design of the course embraces distributed technologies at every level. Student projects are produced by teams, and each member has a well-defined role as manager, programmer, artist, or audio designer. The organization of these teams spans the virtual classroom, and students from LSU are matched in groups of four or five with students in Chicago. In this context, the distributed nature of the course reaches beyond the walls of the classroom. Students must apply networking technologies to all aspects of their work, using online tools for communication, project management, source code synchronization, and file sharing.

In addition to the presentation of this course, forward-looking technologies form the backbone of the content. Students' creative thinking skills are stretched as they are tasked with designing interactive content for unfamiliar platforms. In 2012, the platform was a 3D, stereoscopic, high-resolution LCD system that forced them to consider issues of stereoscopy and scale. The 2011 course used the emerging 4K cinema platform, requiring a thorough consideration of how interactive design and technology changes with a very high density of pixels on screen. The 2010 and 2009 course used the TacTile multi-touch table, asking students to take the familiar touch interface of their cell phone and translate the experience to a multi-user display system the size of a desk. In each case, identical installations of these technologies are available in both Baton Rouge and Chicago, and coordinated use of them is necessary for both out-of-class design and in-class demonstration.

The value of the virtual classroom for a course involving team-based project development is difficult to overstate, as distributed collaboration increasingly reflects the realities of the working world. While today's students are extremely well-versed in casual uses of online technologies, they are often not prepared to deal with the realities of getting work done with these tools. Immersion in collaborative distributed environment adds a new facet to the complete learning experience.

CCT PARTNERS WITH VIRTUAL SCHOOL OF COMPUTATIONAL SCIENCE AND ENGINEERING

For the fourth year, CCT has partnered with the Virtual School of Computational Science and Engineering (VSCSE) to provide training to young professionals from all disciplines, preparing them to use emerging petascale (and then exascale) computing resources to advance their research. Courses include: science cloud; proven algorithmic techniques for many-core processors; programming heterogeneous parallel computing systems; petascale programming environments and tools; and big data for science. CCT has been involved in this initiative since its beginning, together with three other leading institutions: the National Center for Supercomputing Applications (University of Illinois at Urbana-Champaign), the National Institute for Computations Sciences (University of Tennessee, Knoxville), and the University of Michigan.

The VSCSE is a national virtual organization whose goal is to develop and deliver a computational science curriculum that accelerates the ability of faculty, staff, and students to use emerging computational resources to advance science and engineering. Developing and delivering appropriate educational resources requires the collaboration of multiple geographically distributed partner sites with the ability to rapidly experiment with new content and forms of pedagogy in response to new opportunities, technical developments, and challenges.

A unique characteristic of the Virtual School is its use of high-definition (HD) videoconferencing technology to assemble a geographically dispersed group of sites (currently up to 10 sites) into a cohesive HD classroom. In doing so, the Virtual School delivers a quality curriculum to a large number of students at a reduced cost.

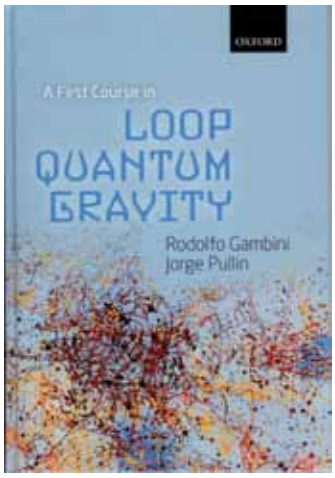
Funding and support for the Virtual School are provided by the Great Lakes Consortium for Petascale Computation, the National Science Foundation, the State of Illinois, the Committee on Institutional Cooperation, and Internet2 Commons.

EXTENDING THE REACH, AFFORDABILITY, AND QUALITY OF EDUCATION!

CCT broadcasts via High Definition (HD) using a life-size video conferencing system to connect to other sites' Tamburg or Polycom systems. Live stream video and audio provide two-way communications along with shared desktop communication allowing instructors and students synchronous collaborations at multiple locations.

Pullin Publishes First Loop Quantum Gravity Text for Undergraduates

LSU's Jorge Pullin, co-director of the Horace Hearne Jr. Institute for Theoretical Physics and professor in the Department of Physics & Astronomy and CCT, recently published a first-of-its kind textbook with the Oxford University Press. Titled *A First Course in Loop Quantum Gravity*, it is the first textbook to cover loop quantum gravity material at the undergraduate level and is based on a course Pullin developed and taught at LSU. Rodolfo Gambini of the University of the Republic of Uruguay is co-author of the textbook.



HPC TRAINING LEVERAGES IMMERSIVE ENVIRONMENTS

HPC@LSU in partnership with CCT offers training in person and via Webcast to the LSU and LONI community on various topics pertaining to use of HPC resources for new and advanced users. Introductory topics are offered such as introduction to HPC and job management as well as advanced topics such as programming/scripting languages, development and debugging tools, and various scientific applications, tools, and visualization. Also conducted are workshops on Fortran and Parallel Programming.

In addition, HPC@LSU and CCT, as a member of the NSF-funded XSEDE project via the Southeastern Universities Research Association, has partnered with the Texas Advanced Computing Center (TACC) to provide training using HD webcast. TACC offers training classes in high performance computing, scientific visualization, basic introduction to using Linux, big data management, distributed and grid computing, and scientific programming in C, C++, and python. Training broadcasts are provided by CCT for the LSU community in person and announcements about TACC training are distributed to the LONI community for participation from their sites.

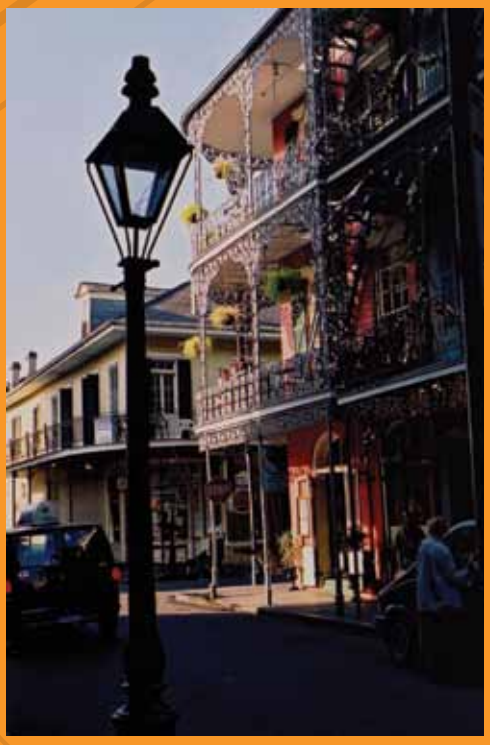
As virtual training gains in popularity, CCT and HPC@LSU will continue to leverage the advantages, bringing world-leaders and their knowledge to LSU and the Louisiana community.

PPOPP'12 HOSTED IN NEW ORLEANS

The 17th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming was hosted in New Orleans, February 25-29, 2012, chaired by J. "Ram" Ramanujam, John E. and Beatrice L. Ritter Distinguished Professor in the LSU Division of Electrical & Computer Engineering.

PPoPP is a forum for leading work on all aspects of parallel programming, including foundational and theoretical aspects, techniques, tools, and practical experiences. In the context of the symposium, "parallel programming" encompasses work on concurrent and parallel systems (multicore, multithreaded, heterogeneous, clustered systems, distributed systems, and large scale machines). Given the rise of parallel architectures into the consumer market (desktops, laptops, and mobile devices), PPoPP is particularly interested in work that addresses new parallel workloads, techniques and tools that attempt to improve the productivity of parallel programming, and work towards improved synergy with such emerging architectures.

Over 200 participants arrived from around the world to share their research, collaborate with other esteemed faculty and researchers, and to visit the New Orleans' historic French Quarter. PPoPP featured tutorials, workshops, a poster session, and technical paper sessions. Proceedings of the symposium are available from the ACM Digital Library.



Cyberinfrastructure

Announcing the Arrival of LSU's Newest Supercomputer:

SuperMike-II

Photo taken by: Phoenix MacAiodh

LSU is pleased to continue its decades-long leadership role in high performance computing with the addition of SuperMike-II to its stable of supercomputing systems. This system introduces two novel capabilities for University researchers: graphical processing unit (GPU) based accelerators and large-memory symmetric multiprocessing (SMP). Its peak performance capability is in excess of 212 TeraFlops (or 212 trillion floating point operations per second).

"SuperMike-II represents the third supercomputer iteration deployed at LSU and provides processing power more than 10 times greater than Tezpur, which was installed in 2007, and 100 times more than LSU's original SuperMike machine, which was launched in 2002," said Honggao Liu, CCT's deputy director and project lead of SuperMike-II. "SuperMike-II provides enhanced support to the current science and engineering user base doing research that ranges from numerical relativity to coastal modeling to molecular dynamics and protein folding. The SMP component will allow new work to be done in the area of graph theory, genome sequencing, and quantum mechanics. The GPU acceleration will be utilized for the design of new materials and new medicines using computational modeling, and advancement of digital media research and production."

SuperMike-II is funded through a joint effort by CCT, Information Technology Services (ITS), and Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA). The $2.6 million system, built by Dell, Inc., features a total of 440 compute nodes (servers), each of which has two Intel Sandy Bridge 8-core processors running at 2.6GHz for a total of 7040 computational cores. The nodes are interconnected by a 40Gbps Mellanox InfiniBand network. While most of the nodes (382) have 32GB of memory, eight are equipped with 256GB each and joined via ScaleMP software to give a single SMP machine with 128 processing cores and 2TB of memory. Fifty nodes are each equipped with 64GB of memory, and two NVIDIA Tesla M2090 GPUs.

Researchers employ supercomputers for complex, large-scale numerical modeling and simulations. These machines use a large number of computational cores, which connect through a high-speed network to run multiple calculations at once or collaborate on a single problem. This new supercomputer's size and speed allow a greater number of elaborate projects to operate simultaneously, according to CCT Director Joel Tohline.

"Our goal is to provide SuperMike-II's services to LSU scientists and engineers who are tackling the most complex problems and require the use of 1,000 or more computational cores at once," said Tohline. "By providing large numbers of GPU accelerators and a symmetric multiprocessor subsystem, entirely new classes of problems can be approached that were totally infeasible before."

Beginning in 2001 with the Flagship Agenda, LSU's strategic vision assigned cyberinfrastructure a central role in research, education, and economic development and includes sustained funding to support CCT. In 2004, this vision was successfully mapped to Louisiana's statewide system of higher education via LONI, the Louisiana Optical Network Initiative—a high-speed, fiber optic network that links supercomputers at the state's six major research institutions, allowing greater collaboration on research that produces results faster and with greater accuracy. SuperMike-II furthers the realization of this vision. It also builds upon the state's construction of a 94,000 square-foot building— the Louisiana Digital Media Center (LDMC)—which, by January 2013, will house the CCT.

"CCT is preparing to move into a new facility, the LDMC," said Tohline. "Through the LDMC, and with the processing power of SuperMike-II, we will encourage new economic development activities by supporting Louisiana's burgeoning digital media production services."

"...we will encourage new economic development activities by supporting Louisiana's burgeoning digital media production services."

CYBERINFRASTRUCTURE— ESSENTIAL TO LOUISIANA'S RESEARCH, EDUCATION, AND ECONOMIC DEVELOPMENT ACTIVITIES

LSU and Louisiana's entire higher education system have adopted and are steadily implementing a strategic vision for cyberinfrastructure, assigning it a central role in research, education, and economic development.

A great opportunity to facilitate implementation of this vision is the $499,758 grant the National Science Foundation recently awarded LSU for CADIS, or more accurately put, a CC-NIE Network Infrastructure— Cyberinfrastructure Advancing Data-Interactive Sciences (CADIS) project.

"CADIS will greatly expand the cyberinfrastructure for the state of Louisiana," said Joel Tohline, director of the CCT. "It will build upon LSU's recent purchase of a new 440-node GPU-enabled High Performance Computing (HPC) cluster and the state's construction of a 94,000 square foot building, the Louisiana Digital Media Center (LDMC), which by January 2013 will house both CCT and EA Sports. The creation of CADIS seeks to integrate tightly the LDMC with the Louisiana Optical Network Initiative (LONI), with LSU's new HPC cluster, SuperMike-II, and with Internet2 (I2)."

The goal of the project is to acquire and install an aggregation router, such as Cisco's ASR 9010, with an appropriate set of cards and adapters in order to do several things. First, to extend the current data transport capabilities of LONI and I2 to researcher desktops and to the LDMC's 4K theatre via dedicated 10 Gbps network connections. Second, to build a 40 Gbps data-transport pipe between LSU's new GPU enabled SuperMike-II cluster and the LDMC's primary visualization laboratory. Finally, to provide straightforward paths for upgrading laboratories and offices to higher bandwidth connectivity as the capabilities of LONI and I2 expand.

The LDMC will gather the University's primary base of HPC users under one roof where, via the activities of the CCT, a unified focus on interactive digital media and HPC is provided. Students, postdocs, research scientists, and faculty from diverse disciplinary backgrounds who seek to harness HPC resources to simulate and/or analyze complex phenomena will effectively collaborate with other researchers who have expertise in scientific computing, the development of HPC algorithms, visualization and image processing, and the manipulation and analysis of large datasets.

"CADIS will create many opportunities for LSU's diverse research community to more effectively interact with huge data sets that are generated on local (LSU), regional (LONI), and national (XSEDE) HPC resources, angling new scientific and engineering discoveries. And, through CCT's collaborative interactions with Louisiana's rapidly growing collection of digital media industries, the CADIS project is expected to positively impact key economic development activities across Louisiana," said Tohline.

The project team includes Honggao Liu, deputy director of CCT and site lead for LONI; James A. Lupo, assistant director of computational enablement at CCT; Lonnie Leger, director of networking at LONI; Brygg Ullmer, associate professor of computer science and CCT; Ric Simmons, deputy CIO and executive director of network infrastructure at LSU; and Sean G. Robbins, director of network engineering, LSU Information Technology Services.

GPU CLUSTER PREPARES LOUISIANA FOR NEXT-GENERATION SUPERCOMPUTERS

CCT recently received $539,999 from the National Science Foundation for "Shelob," a computer cluster to be used for computer science research, education, training, and development for Louisiana. Shelob is a system composed of multiple server nodes—commonly called a Beowulf cluster—but each node will include graphical processing units (GPUs) to add additional processing power. The Shelob GPU cluster will include at least 24 compute nodes, one head/control node, and 100 terabytes of scratch disk storage. The nodes will communicate with each other over a Fourteen Data Rate InfiniBand network fabric at a data rate of 56Gb/s. Each node will have at least 64GB of memory, dual 8-core Intel Sandy Bridge processors, and three next-generation NVIDIA "Kepler" GPUs. The Shelob cluster will be used primarily to develop a large set of open source GPU-enhanced research applications.

"We propose to transform computer and computational science research and education throughout Louisiana by graduating our users from the current massively parallel paradigm to a GPU-enabled parallel paradigm," said Honggao Liu, deputy director of the CCT. "To use the next generation of GPU-accelerated national leadership supercomputers that will come on-line over the next couple of years, researchers will need to write GPU-enhanced massively parallel codes. The payoff from this project will be significant. Hundreds of researchers throughout Louisiana will use the Shelob cluster to develop a new generation of codes to use these new supercomputers."

CCT NAMED 2012 CUDA RESEARCH CENTER BY NVIDIA

NVIDIA, the world leader in visual and high performance computing, selected CCT as a 2012 CUDA Research Center. The designation recognizes CCT's research using CUDA to streamline heterogeneous system programming, which utilizes both GPU and CPU processors within a computing system.

"CCT's advancements in CUDA and GPU computing applications are in line with Louisiana's Digital Media and Software Initiative and have played an important role in attracting major companies such as Pixomondo and Electronic Arts, which chose LSU as the site of its first North American Test Center in 2008," said Honggao Liu, CCT's deputy director. "A CUDA Research Center on campus will help establish industry partnerships with digital media and software companies to work on CUDA-based projects as well as help prepare students for careers in these fields."

CUDA is NVIDIA's parallel computing platform that enables dramatic increases in computing performance by harnessing the power of the GPU. CUDA is currently being taught in more than 580 universities and institutions around the world, and CUDA Research Centers, which are at the forefront of some of the world's most innovative and important scientific research, are recognized institutions that embrace and utilize GPU computing across a range of research fields. The CUDA Research Center Program gives CCT access to benefits such as the latest NVIDIA products and the opportunity to interact with computing industry experts from around the world.

Photo taken by: Jim Zietz, LSU Office of Communications & University Relations

ECONOMIC DEVELOPMENT

"Louisiana's software and digital media sector is taking off, with companies like Ameritas Technologies, CenturyLink, Gameloft, GE Capital, Pixomondo, Schumacher Group, TraceSecurity, TurboSquid and others collectively planning to add many hundreds of computer science grads over the next few years."
–Gov. Bobby Jindal, 2012

CHANGING LOUISIANA'S TOMORROW THROUGH TECHNOLOGICAL ADVANCES

It is fair to say that the CCT stumbled into its role as a significant player in both Baton Rouge's and Louisiana's economic development efforts. In the CCT's 2006 – 2010 Strategic Plan, the economic development objectives stress "technology transfer," "contact with entrepreneurs," "cooperative agreements," and "encouraging the use of new and improved technologies in the marketplace."

In practical terms, what worked was the Red Stick International Animation Festival (RSIAF)! The RSIAF was largely the brainchild of Stephen Beck and Stacey Simmons—two CCT leaders—and, as is affirmed on the BRADIC Web site, the Baton Rouge Area Digital Industries Consortium was founded on the success of the RSIAF.

EA Sports, Pixomondo, and other video game and digital media companies have moved a portion of their worldwide operations to Baton Rouge, in part, because they anticipated reaping benefits from collaborative interactions with the CCT's faculty, staff, and students. Sufficient faith is being put in the potential for collaborative interactions between EA and the CCT that the LSU Research Foundation is building a new building—the Louisiana Digital Media Center—near the south gate of LSU to jointly house EA and the CCT. (See the related article in last year's *Components*.) Our move to this new building should happen early in 2013.

Through our interactions with the state (Louisiana Economic Development (LED)) and the city (Baton Rouge Area Chamber (BRAC) and Baton Rouge Area Foundation (BRAF)), it has become abundantly clear that workforce training is a critical issue that arises in all discussions with companies that consider moving all or part of their operations to Louisiana. This issue resonates with CCT. Our desire to build a strong, interdisciplinary digital media research program at LSU has resulted in the development of the AVATAR initiative and two key educational programs. Video game and visual effects companies view these educational programs as a prime training ground for the skilled workforce that they need. Because the city, state, and private industry are very interested in the success of our proposed graduate-level Digital Media Arts and Entertainment (DMAE) program in particular, representatives from LED, BRAC, and BRAF have been invited and have agreed to serve this year on our committee charged with recruiting and hiring the DMAE program director.

Over the past year the CCT has led the University's effort to acquire a new HPC system to support challenging computational modeling and data analysis efforts across a wide range of science and engineering disciplines. As we were deciding on the architectural design of this new HPC system during the 2010/11 academic year, we also explored the possibility that the HPC system might be used to directly support Louisiana's economic development efforts. We proposed an HPC business model that now has LSU's full support. The key element of the proposal is that LSU should make the new supercomputer's resources available as a render farm to visual effects (VFX) artists who work in Louisiana. Even if the level of demand and usage by the commercial VFX community is as little as 10 percent of the HPC system's available compute cycles, in three years the resulting revenue stream would go a long way toward covering the costs of a new, replacement HPC system. Hence, CCT expects a double win: we can assist the state's economic development efforts and, simultaneously, help ensure sustained support for LSU's computational sciences research programs.

> **"LSU should make the new supercomputer's resources available as a render farm to visual effects (VFX) artists who work in Louisiana."**

Over the coming year, the CCT anticipates continued expansion of, and benefits from, its ties with Louisiana's economic development efforts.

Lagniappe

HIGHLIGHTS 2012

Jorge Pullin, CCT and LSU Department of Physics & Astronomy, has been appointed to the advisory board of the open access journal *Papers in Physics*, the only journal in physics to offer open peer review.

CCT's **Peter Diener** et al. were published in *Physical Review Letters*, one of the world's most prestigious publications in physics, providing coverage on major advances in physics and cross disciplinary developments.

Susanne Brenner, CCT and LSU Department of Mathematics, was a plenary speaker at the 36th Annual SIAM Southeastern Atlantic Section Conference at the University of Alabama in Huntsville. Her talk was titled "Finite element methods for a fourth order obstacle problem."

CCT's **Christian Ott** received a Sloan Research Fellowship awarded to early-career scientists and scholars whose achievements and potential identify them as rising stars, the next generation of scientific leaders.

The **Cactus group** at CCT announced the fifth release of the Einstein Toolkit, an open, community developed software infrastructure for relativistic astrophysics.

Susanne Brenner was appointed by the Council of the American Mathematical Society as managing editor of *Mathematics of Computation.*

Michael Khonsari, CCT and LSU Department of Mechanical Engineering, was honored with the rank of "Fellow" by the American Association for the Advancement of Science, the world's largest scientific organization. Khonsari was honored for his distinguished contributions to multidisciplinary scientific research and development, particularly in the field of tribology, and for outstanding leadership in building research infrastructure across the state of Louisiana.

Jorge Pullin recently published a textbook with the Oxford University Press and co-author Rodolfo Gambini of the University of the Republic of Uruguay. Titled *A First Course in Loop Quantum Gravity*, it is the first textbook to cover the loop quantum gravity material at the undergraduate level and is based on a course Pullin developed and taught at LSU.

CCT's scientific visualization researcher, **Werner Benger**, had a black hole image selected for the cover of the October 2011 issue of *Physics World*. He also won the CASC (Coalition for Academic Scientific Computation) image competition, and his stirred tank reactors image will appear on the cover of CASC's 2012 brochure.

Ram Ramanujam, CCT and LSU Division of Electrical & Computer Engineering, was appointed as general chair of the 17th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming (PPoPP 2012), which was held in New Orleans, Louisiana.

Susanne Brenner was one of the plenary speakers at the International Conference on Computational Sciences, which was held July 16-20, 2012, at the Shanghai Normal University in Shanghai, China.

Robert Lipton, CCT and LSU Department of Mathematics, has been appointed to the Editorial Board of the SIAM *Journal on Mathematical Analysis.*

Physical Review X, the journal of which **Jorge Pullin** is founding editor, has been shortlisted for best journal of the year by the Association of Learned and Professional Society Publishers.

Susanne Brenner was appointed to the Scientific Committee of the Basque Center for Applied Mathematics in Bilbao, Spain.

LSU teams at the CCT and the LSU School of the Coast & Environment have developed a sophisticated, interactive, and dynamic Web interface titled Coastal Emergency Risks Assessment, or CERA, providing operational advisory services related to impending hurricane events and other coastal hazards. The teams are lead by **Harmut** and **Carola Kaiser**, both IT professionals at the CCT.

FACULTY PROMOTIONS AND OTHER LSU HONORS:

Gabrielle Allen was promoted to full professor in the Division of Computer Science & Engineering.

Q. Jim Chen was promoted to full professor in the Department of Petroleum Engineering and named first CSRS Distinguished Professor in Coastal Engineering.

Juana Moreno received tenure and was promoted to associate professor in the Department of Physics & Astronomy.

Lance Porter received the Mary P. Poindexter Professorship in the Manship School of Mass Communication.

Georgios Veronis received the Charles Siess Jr. Distinguished Professorship in the Division of Electrical & Computer Engineering.

Proven Algorithmic Techniques for Many-core Processors, Virtual School
Dates: August 15-19, 2011
Attendees: 18
Location: LSU

ACM Regional Programming Contest
Dates: October 28-29, 2011
Attendees: 66 teams across four sites
Locations: LSU, Baylor University, LeTourneau University, East Central University

CCT 10-Year Anniversary Celebration
Date: October 26, 2011
Attendees: 125
Location: LSU

Red Stick International Animation Festival Fall Retrospective
Date: November 10, 2011
Attendees: 450
Location: Shaw Center for the Arts, Baton Rouge

3rd Annual Scientific Computing around Louisiana Workshop
Dates: January 20-21, 2012
Attendees: 74
Location: LSU

18th Annual Mardi Gras Conference on Computational Materials & Biosystems
Dates: February 16-18, 2012
Attendees: 75
Location: LSU

ACM Symposium on Principles and Practice of Parallel Programming
Dates: February 25-29, 2012
Attendees: 220
Location: Hotel Monteleone, New Orleans

"Perception" Premiere—Laptop Orchestra of Louisiana
Dates: March 10, 2012
Attendees: 75
Location: Shaw Center for the Arts, Baton Rouge

NanoDays in Baton Rouge
Dates: March 24, March 31, 2012
Attendees: 175
Locations: Louisiana Art & Science Museum and Highland Road Park Observatory

Inaugural Symposium on Laptop Ensembles & Orchestras
Dates: April 15-17, 2012
Attendees: 100
Location: LSU

Research Experience for Undergraduates 9-week programs (computational sciences and LASiGMA-materials science)
Dates: May 29-July 28, 2012
Attendees: 37 selected from 167 applicants
Locations: LSU, LA Tech, Southern University, Tulane University, and Xavier University

Research Experience for Teachers (LASiGMA-materials science)
Dates: May 29-July 28, 2012
Attendees: 17
Locations: LSU, LA Tech, Southern University, and Tulane University

LONI HPC Parallel Programming Workshop
(Louisiana Optical Network Initiative)
Dates: June 4-6, 2012
Attendees: 25
Location: LSU

HPC Users' Symposium
Dates: June 6-8, 2012
Attendees: 100
Location: LSU

7th Red Stick International Animation Festival & "Best of the Fest" Competition
Dates: June 8-10, 2012
Attendees: 900
Location: Shaw Center for the Arts, Baton Rouge

NWChem Workshop
Dates: June 11-13, 2012
Attendees: 25
Location: LSU

2nd Alice in Computation Land Summer Camp for Middle School Girls
Dates: June 18-22, 2012
Attendees: 22
Location: LSU

5th Beowulf Boot Camp for High School Students & Teachers
Dates: July 9-13, 2012
Attendees: 43
Location: LSU

Programming Heterogeneous Parallel Computing Systems Workshop, Virtual School
Dates: July 10-13, 2012
Attendees: 19
Location: LSU

iOS Application Boot Camp for LSU Undergraduates
Dates: July 30-August 10, 2012
Attendees: 23
Location: LSU

Science Cloud Summer Workshop, Virtual School
Dates: July 30-August 3, 2012
Attendees: 5
Location: LSU

Lectures 2011-2012
Sponsored by CCT and held at LSU
Speakers Fall 2011 through Summer 2012: 43 total

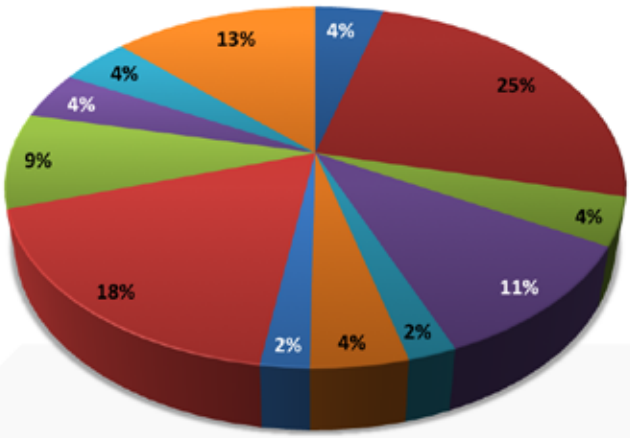
Lectures by Category:
CCT Distinguished—1
CCT Tech Talk Series—4
Special Guest Lectures—15
Computational Mathematics Seminar Series—17
AVATAR (Arts, Visualization, Advanced Technologies and Research) Lecture Series—3
Frontiers of Scientific Computing—3

High-Performance Computing Tutorials 2011-2012
Held at LSU
Organized by CCT and HPC @ LSU

Fall 2011: 10 tutorials
Spring 2012: 11 tutorials
Summer 2012: 2 tutorials

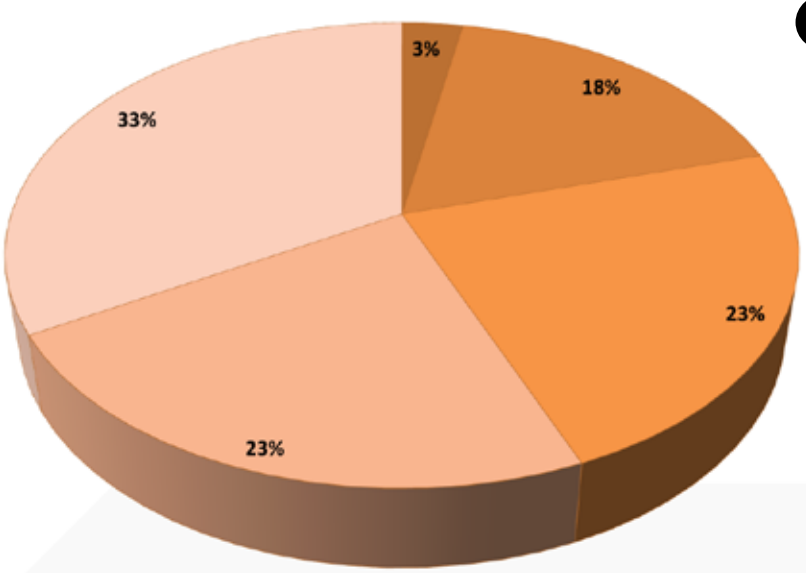
BUSINESS REPORTS

CCT FACULTY BY DEPARTMENT 2012



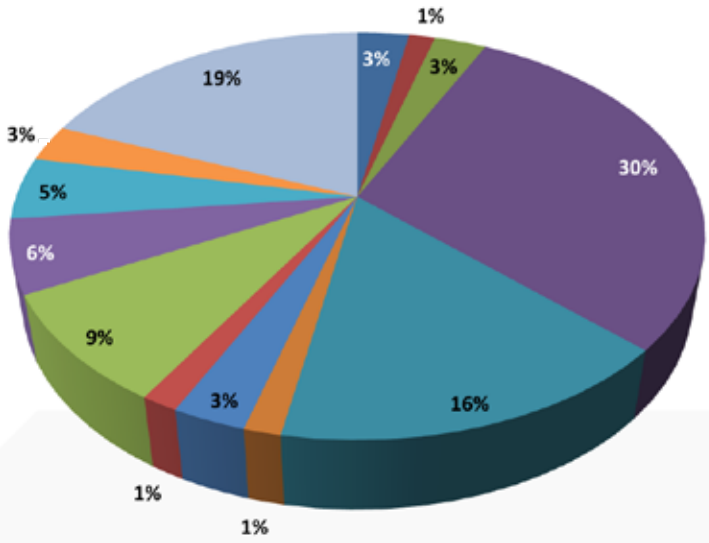
- Art & Design 4%
- Computer Science 25%
- Chemistry 4%
- Electrical & Computer Engineering 11%
- Enviromental Engineering 2%
- Information Systems and Decision Science 4%
- Mass Communication 2%
- Mathematics 18%
- Mechanical Engineering 9%
- Music 4%
- Petroleum Engineering 4%
- Physics & Astronomy 13%

CCT PROFESSIONAL STAFF 2012



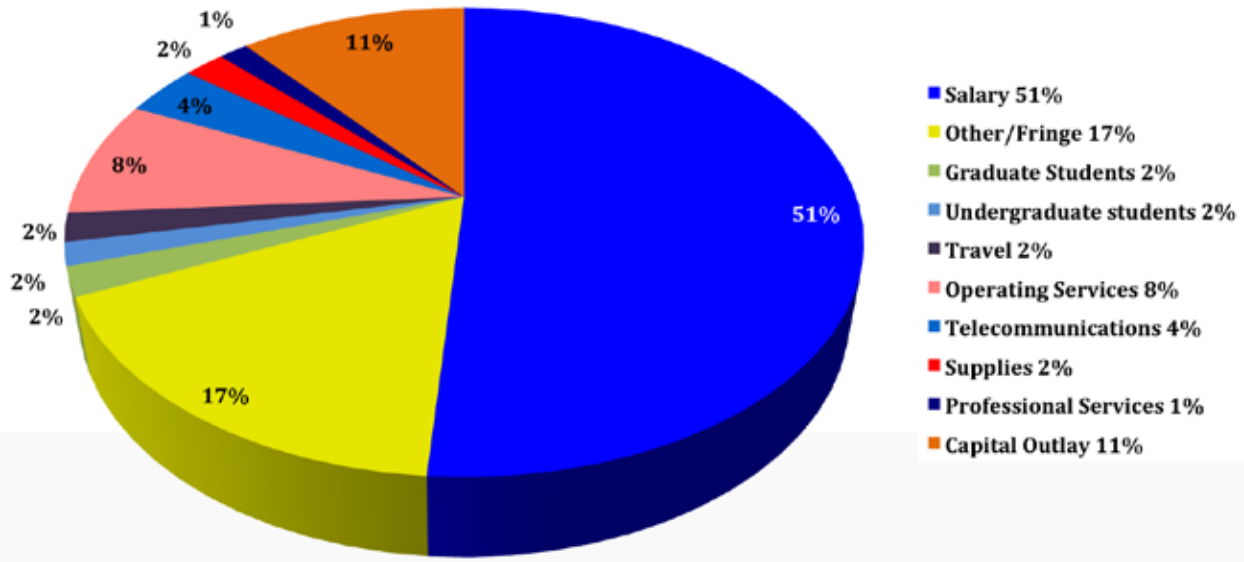
- Economic Development & Digital Media Staff 3%
- Executive & Administrative Staff 18%
- Technical Staff 23%
- Postdoctoral Researchers 23%
- Research Scientist 33%

CCT GRADUATE ASSISTANTS BY DEPARTMENT 2012

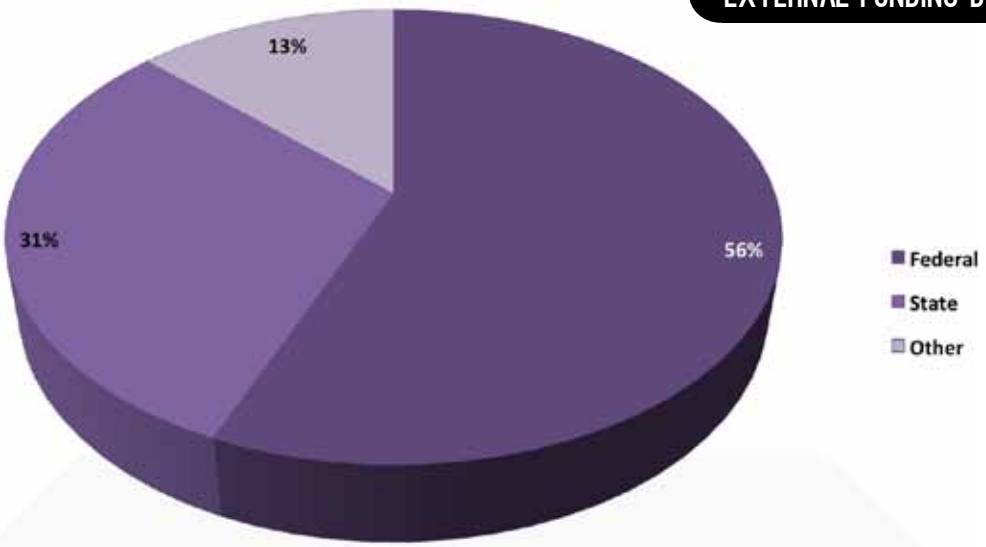


- Art 3%
- Chemical Engineering 1%
- Chemistry 3%
- Computer Science 30%
- Electrical & Computer Engineering 16%
- English 1%
- Information Systems & Decision Sciences 3%
- Library & Info Sciences 1%
- Mathematics 9%
- Mechanical Engineering 6%
- Music 5%
- Petroleum Engineering 3%
- Physics 19%

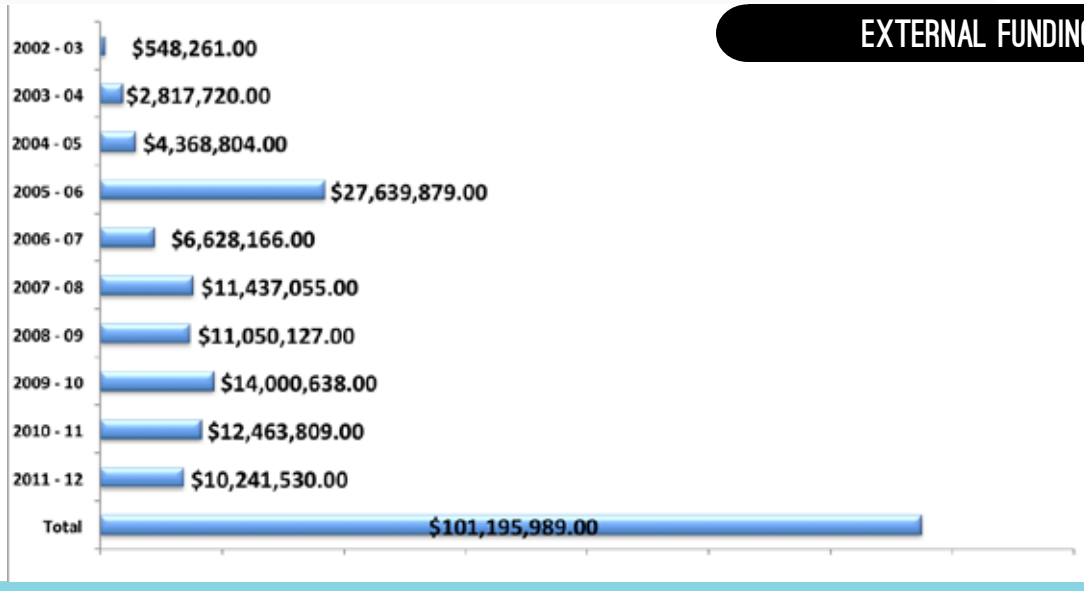
CCT INVESTMENT SUMMARY 2011-2012



EXTERNAL FUNDING BY SOURCE FOR FY 2003-2012



EXTERNAL FUNDING FY 2003-2012



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