LONI Institute Fourth Annual Report
PKSFI Project
July 1, 2010 – June 30, 2011

Principal Investigator: Mark Jarrell, LSU

Scientific Coordinator: Bety Rodriguez-Milla, LSU

Projects Committee Lead: Shantenu Jha, LSU

Co-Principal Investigators:

Louisiana State University	Tevfik Kosar, Steven Soper
Louisiana Tech University	Les Guice, Chokchai Leangsuksun, Bala (Ramu) Ramachandran, Neven Simicevic
Southern University at Baton Rouge	Michael Stubblefield, Ebrahim Khosravi, Habib Mohamadian
Tulane University	Gary McPherson, Ricardo Cortez, Lisa Fauci, Donald Gaver
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University of New Orleans	Scott Whittenburg, Vassil Roussev, Stephen Winters-Hilt

Website: http://institute.loni.org

I. INTRODUCTION

The LONI Institute is part of a coordinated effort to improve computational sciences research and education throughout the state of Louisiana. The three pillars of this project are the LONI network, the LONI Institute and the recent NSF LA-SiGMA award. The LONI network provides the high-speed connections required to connect this statewide virtual graduate research and education project. It also provides the computational resources. The LONI Institute provides the resources to hire the requisite computational sciences faculty and staff. The LA-SiGMA award recently secured by LONI Institute faculty is the third pillar. It provides funding that supports LONI Institute researchers and their research groups. LONI Institute and LA-SiGMA allow these researchers to leverage the LONI hardware in their research and to train the next generation of computational scientists for Louisiana.

In its fourth year, LONI Institute has grown dramatically in both its impact and its research productivity, and is moving forward toward its goal of establishing a statewide virtual institute in the computational sciences. Changes this year include:

- The award of the LONI Institute spinoff project: *The Louisiana Alliance for Simulation-Guided Materials Applications (LA- SiGMA): Leveraging Next Generation Supercomputing for the Study of Complex Multiscale Phenomena in Materials, 9/1/10—8/31/15:* EPS-1003897. This $20M award funds a statewide virtual graduate research and education project in computational materials science.
- With this award, the total federal funding raised by LONI Institute researchers now exceeds $35M.
- The LONI Institute seminar series. Every two weeks throughout the school year leading researchers visit one of the LONI Institute campuses and deliver a talk that is shared with the other campuses via synchronous video.
- LONI Institute courses. LONI Institute faculty teach several specialized courses in various computational sciences topics. These courses are shared with all LONI Institute campuses via synchronous video.
- LONI Institute training workshops. The LONI Institute is the main sponsor or co-sponsor of a number of workshops that provide advanced training in the computational sciences. These include training in parallel computing, workshop on density functional theory, and the well-known Beowulf Boot Camp.
- LONI Institute members at ULL are in the final stages in the development and approval of an NSF Center on Visual and Decision Informatics (CVDI), a planned Industry-University Cooperative Research Center.

The impact of the LONI Institute is significant. During very difficult economic times, it has allowed Louisiana Institutions to hire leading researchers in the computational sciences. These researchers have attracted a significant amount of funding which is being used to train a new generation of computational sciences researchers who will sustain the Institute into the future.

This report follows the requisite format. In the next section, II, the personnel hired by or working with the LONI Institute are listed. In section III, the activities and finding of the LI researchers are detailed. This section ends with a discussion of the LONI Institute seminars, courses, and workshops. In section IV we provide a brief summary and in section V we discuss changes to the project.

II. PERSONNEL

List all key personnel and other staff who provided significant contributions to the project. Provide information about the types of contributions made by each listed participant and controls in place to ensure that these contributions are adequate to the project's requirements.

The LI key personnel can be divided into LI Faculty, LI Computational Scientists, LI Graduate Fellows, LI Senior Investigators, and LI Staff. Please see the personnel before.

LI Faculty.

* Dr. Scott Duke–Sylvester, Assistant Professor, Department of Biology, University of Louisiana at Lafayette (ULL).
* Dr. Dentcho Genov, Assistant Professor, Department of Physics and Electrical Engineering, Louisiana Tech University (LA Tech).
* Dr. Mark Jarrell, Professor, Department of Physics & Astronomy, Louisiana State University (LSU).
* Dr. Damir Khismatullin, Associate Professor, Biomedical Engineering Department, Tulane University (Tulane).
* Dr. David Mobley, Assistant Professor, Chemistry Department, University of New Orleans (UNO).
* Dr. Zhenyu Ouyang, Assistant Professor, Department of Mechanical Engineering, Southern University at Baton Rouge (SUBR).
* Dr. Caz Taylor, Assistant Professor, Department of Ecology and Evolutionary Biology, Tulane.
* Dr. Christopher Taylor, Assistant Professor, Department of Computer Science, UNO.
* Dr. Rachel Vincent-Finley, Assistant Professor, Department of Computer Science, SUBR.
* Dr. Collin Wick, Assistant Professor, Department of Chemistry, LA Tech.

LI Computational Scientists

Dr. Hideki Fujioka, Center for Computational Science, Tulane
Dr. Raju Gottumukkala, Center for Business, and Technology (CBIT), and National Incident Management Systems and Advanced Technologies (NIMSAT), ULL
Dr. Abdul Khaliq, Institute for Micromanufacturing (IfM), LA Tech
Dr. Bhupender Thakur, Center for Computation & Technology, LSU
Dr. Shizhong Yang, Computer Science Department and College Engineering, SUBR
Dr. Zhiyu Zhao, College of Sciences, UNO

2010 LI Graduate Fellows

Mr. Murat Seckin Ayhan, Center for Advanced Computer Studies (CACS), ULL
Mr. Shravanrakesh Animilli, Department of Physics, LA Tech
Mr. Corey Baham, Department of Computer Science, SUBR
Mr. Lide Duan, Department of Electrical and Computer Engineering, LSU
Mr. Elliott James, College of Engineering and Science, LA Tech
Mr. Derrick Goss, Department of Mechanical Engineering, SUBR
Ms. Jerina Pillert, Biomedical Engineering Department, Tulane
Ms. Shanshan Shen, Mathematics Department, Tulane
Mr. Guorong Xu, Department of Computer Science, UNO
Mr. Hongtao Yu, Department of Chemistry, UNO
Ms. Ashley Zebrowski, Department of Computer Science, LSU
Mr. Haochun Zhang, Mathematics Department, ULL

LI Senior Investigators

Dr. Ricardo Cortez, Associate Professor, Mathematics Department, Tulane
Dr. Weizhong Dai, Professor, Mathematics Department, LA Tech

Dr. Pedro Derosa, Associate Professor, Department of Physics and IfM at La Tech, and Grambling State University (GSU)
Dr. Sumeet Dua, Assistant Professor, Department of Computer Science, LA Tech
Dr. Lisa Fauci, Professor, Mathematics Department, Tulane
Dr. Donald Gaver, Professor, Department of Biomedical Engineering, Tulane
Dr. Z. Dick Greenwood, Associate Professor of Physics, LA Tech
Dr. Shantenu Jha, Center for Computation & Technology, and Department of Computer Science, LSU
Dr. Ebrahim Khosravi, Professor, Computer Science Department, SUBR.
Dr. Ramesh Kolluru, Executive Director, NIMSAT, Director, CBIT, ULL
Dr. Daniela Mainardi, Assistant Professor, Department of Chemical Engineering, LA Tech
Dr. Juana Moreno, Department of Physics & Astronomy, LSU
Dr. Ramu Ramachandran, Professor, Department of Chemistry, LA Tech
Dr. Neven Simicevic, Assistant Professor, Department of Physics, LA Tech
Dr. Scott Whittenburg, Professor, Chemistry Department, UNO

LI Staff
Ms. Shelley Lee, Part-time Project Coordinator
Dr. Berta Rodriguez-Milla, Scientific Coordinator

III. ACTIVITIES AND FINDINGS

A) Describe major research and educational activities undertaken in this reporting period;
B) Describe and provide data supporting the major findings resulting from these activities;
C) Describe the opportunities for faculty recruitment, retention and development, as well as post-doc, graduate and undergraduate student training provided by your project;
D) Describe the nature and scope of partnership activities; and
E) Describe any problems encountered during the last year of project activities.

A, B) Major research and educational activities

LI Faculty

Dr. Scott Duke–Sylvester, ULL, Spatial and Theoretical Biology

Research Group Members: Nicholas Treusch. Graduate Student, Department of Biology

Research Projects

Revealing signatures embedded within rabies virus phylogeny produced by the demography of host/pathogen interactions.

Ecological and evolutionary analyses have largely remained separate with different intellectual communities undertaking one or the other form of analysis, but rarely both. Often, the obstacle to combined analysis resides in an apparent large difference in the time-scale of operation of evolutionary and ecological processes (millennia versus months or years). Yet, for many host-pathogen systems, especially those associated with RNA viral pathogens, the time-scale of ecological dynamics and evolutionary change are identical. A focus on the combined ecological-evolutionary dynamics of RNA viruses not only provides a key for uniting these disparate intellectual fields, but also is particularly prescient since most (~75-85%) emerging pathogenic threats to human health are associated with RNA viruses.

My research on infectious disease is focused on analyzing the phylogenetic structure of a pathogen to reveal the unobserved dynamics of an epidemic. I am actively developing a model to simulate the molecular evolution of the rabies virus linked to the spatial epidemiological dynamics of rabies spread. Using this model, I am examining how spatial heterogeneity in different aspects of host demography change phylogeny of the pathogen. Preliminary results from this model, calibrated for the spread of raccoon rabies, suggest that spatial heterogeneity in the host carrying capacity produces a quantitatively different phylogeny pattern for rabies than does spatial heterogeneity in the dispersal of raccoons between locations. My goal is to establish a mechanistic explanation that relates observed phylogeny patterns in pathogen diversity to the ecological processes that influenced disease dynamics. This framework could be used to provide insights into the spatial ecology of the host population and can be used to direct efforts to control the disease. Future research in this area includes examining the role of additional aspects of host demography including age structure, seasonality as well as incorporating the effects of landscape features such as mountains and urbanized areas. Future projects will also extend the model to multi-host systems as well as considering vector born diseases. An advantage to using rabies in this research is the neutral molecular evolution of the target genes that permits a relatively straightforward evolutionary model. A more ambitious and longer-term project is to begin modeling the interaction between pathogen evolution and host dynamics in the presence of positive selection on the pathogen.

My research on the ecology and evolution of the rabies virus is of both direct public health importance and has the potential to have broader impacts. Rabies infection in both people and animals is the only zoonosis that must be reported the US Centers for Disease Control and Prevention (US-CDC). While there are only a few confirmed cases of human rabies infection each year, control of rabies in the United States still exerts a tremendous annual cost estimated at over $300 million in vaccination and prevention and an additional $30 million in post exposure prophylaxis of some 35,000 – 40,000 persons with suspected infections. Assessing the effectiveness of programs targeted at controlling wildlife rabies is hampered by the difficulties associated with monitoring wildlife populations. Wildlife trapping efforts are expensive and often there are insufficient samples collected at any give time or place to provide an accurate estimate of the infection status of the population based on standard techniques of demographic analysis. However, analysis based on the viral RNA can reveal important features of an epidemic based on the limited sampling data that is available.

My research can also be applied to a range of other pathogens of major public health concern. Many infectious diseases that infect humans, including influenza, measles and Ebola are RNA viruses with rapid rates of molecular substitution and evolve at a rate compatible with their rate of spread. My research can readily be applied to provide insights into the patterns of spread during emerging epidemic or pandemic events. Revealing these patterns can help guide the allocation of public health resources and inform the implementation of public health policies, such as travel or importation bans that are effective while avoiding excessive disruption to the economy.

The landscape ecology of coastal and wetland ecosystem of the southeastern United States.

The Everglades is a case study in the dynamic tension between a natural environment and its exploitation by man. The ecosystem is characterized by a unique assemblage of plant communities including grass-dominated fresh-water marshes, tree islands, coastal mangrove forests and cypress swamps and is host to distinctive community of animals including several endemic and endangered species. During the 20th century the human population of Florida increased from less that 600,000 to more that 15 million people {US Census Bureau}. To support the activities of the urban population an extensive system of water control structures was constructed to provide flood control and exploit the Everglades' vast freshwater resources. The water control system compartmentalizes the once continuous sheet flow of water. Further the management of water for human use has lead to unnatural distributions of water within the Everglades

including increases in water depths and hydroperiods beyond natural levels and producing drought conditions out of the historical dry season.

My research is focused on how future management of freshwater will change the Everglades plant communities. Addressing the question is a non-trivial task given the mechanisms through which plants respond to their environment, the numerous hydrologic changes proposed to effect restoration goals, and the spatial extent of the ecosystem. My approach to handling the complexities that underlie our question is to apply a simulation model. The simulation model I have developed simulates shifts between the dominant Everglades vegetation types in response to changes in hydrology.

I am also extending my research to the plant community dynamics of coastal Louisiana. The unique ecosystem has been significantly disturbed by years of human intervention. The Louisiana Office of Coastal Protection and Restoration (LOCPR) has initiated a concerted effort to restore the coastal ecosystem of Louisiana over the next 50 years. This effort involves a number of individual projects restoration projects. To help evaluate the relative impact of these different projects and guide their implementation the LOCPR has commissioned a broad modeling effort designed to evaluate the effect of restoration projects on the hydrology, soil morphology, storm surge/wave risk, fauna and flora of coastal Louisiana. My participation in this larger project is to develop a computational model of plant community dynamics. This model will simulate the effects of restoration projects on coastal plant communities and will be used to refine and update the implementation of these projects.

Publications

- **Duke-Sylvester, S.M.**, Bolzoni, L., Real, L.A. (2011). Strong seasonality produces spatial asynchrony in the outbreak of infectious diseases. Journal of the Royal Society Interface. 8:817-825
- Clayton, T., **Duke-Sylvester, S.M.**, Gross, L.J., Lenhart, S., Real, L.A. (2010). Optimal control of a rabies epidemic model with a birth pulse. Journal of Biological Dynamics. 4:43-58.

Presentations/Talks

- July, 2010. Louisiana Optical Network Initiative (LONI) 2010 Summer Workshop for Louisiana High School Teachers, Baton Rouge, LA. Title: Rabies in Space.
- October, 2010. Biology Department Seminar, University of Louisiana at Monroe, Monroe, LA. Title: Rabies in Space.
- March, 2011. Louisiana Immersive Technologies Enterprise (LITE). CAVE Fellow talk. Title: Rabies in Space.

External Funding

- Vegetation Modeling for Coastal Louisiana Wetland Ecosystems
  PI: Jenneke Visser, Department of Renewable Resources, University of Louisiana at Lafayette
  Source of Support: Louisiana Office of Coastal Protection and Restoration
  Total Award Amount: $ 149,299
  Status: Funded
- Integrating ecological and evolutionary theory to understand the epidemiology of rapidly evolving viral pathogens.
  PI: Scott M. Duke-Sylvester, Department of Biology, University of Louisiana at Lafayette
  Source of Support: Louisiana Board of Regents
  Support Fund Total Award Amount: $ 113,985
  Status: Funded

Recent Applications for External Funding

- Collaborative Research: Modeling the population ecology and genetics of Amblyomma maculatum ticks
  PI: Holly Gaff, Department of Biology, Old Dominion University, Norfolk, VA
  Source of Support: National Science Foundation
  Total Award Amount: $ 674,521
  Status: Pending
- FESD Type II: A Delta Dynamics Collaboratory
  PI: David Mohrig, Department of Geology, University of Texas at Austin, Austin, TX
  Source of Support: National Science Foundation
  Total Award Amount: $ 1,200,000
  Status: Pending
- What are the effects of nutrient loading on marsh accretion rates in a changing climate?
  PI: Jenneke Visser, Department of Renewable Resources, University of Louisiana at Lafayette
  Source of Support: Sea Grant
  Total Award Amount: $254,470
  Status: Pending

Dr. Dentcho Genov, LA Tech, Electromagnetic Metamaterials and Nanophotonics

Research Group Members:

Venkatesh Kumaran, PhD student (theory/computation)
Pattabhiraju Mundru, PhD student (theory/computation)
Shravan Rakesh Animilli, PhD student (theory/computation)
David C. Hertlein Jr., MS student (theory)
Mona Saleh, MS student (theory and experiment)

Research Interests

- Electromagnetic properties of nano-structured complex media including: metal composite materials, rough surfaces, fractal aggregates, and ordered media
- Solid state and condensed matter physics: geometrical phase transitions, scaling theory, classical and quantum wave localization phenomena
- Nanophotonics and quantum optics, nonlinear optics and spectroscopy, quantum dots, nanoscopic lasers and optical elements, light scattering from metal particles
- Artificial materials: metamaterials and negative index media, electric and magnetic plasmon waveguides, plasmonic and ordinary band gap materials
- Numerical code development and algorithm optimization, large-scale computer simulations in electrodynamics, plasma physics, and material science

Research Projects

The main focus of our research is a rapidly developing field of artificial optical materials, referred to as electromagnetic metamaterials (EMMs). The phenomenal progress in nanofabrication now provides the enabling technology to develop EMMs with unlimited range of optical properties opening the possibility to manipulate light at will. This is accomplished by precise engineering of the microscopic magnetic and electric response of the media and is equivalent to virtually creating *new* types of quasi-atoms and quasi-molecules. The EMMs have been proposed for negative refractive index media, invisibility devices and lenses with super resolution. The LI faculty (Genov) has substantially contributed to this field publishing more than 40 papers in top peer reviewed journals and conference proceedings, including; *Nature*, *Nature*

Physics, *Nature Photonics*, *Phys. Rev. Lett.*, etc. Currently my group is working on the following six research projects:

a. Computational engineering of EMMs for optical invisibility (a PhD student involved)
b. Numerical methods in nanoplasmonics: electrodynamics of disordered electromagnetic media (a PhD student and LI CS (A. Khaliq) involved).
c. Surface Plasma Enhanced Solar Cells (SPESC) (a PhD student involved).
d. Surface Plasmon based THz transistor (a PhD students and LI CS (A. Khaliq) involved).
e. Reversal of Casimir force in Metamaterials: (a PhD student involved).
f. Continuous Index Photon Traps (CIPT) (a MS student involved)

a. Computational engineering of EMMs for optical invisibility: Cloaking is an advanced stealth technology that utilizes EMMs to render objects invisible from arbitrary electromagnetic fields. The most popular methods for achieving invisibility are based on encapsulating the object in EMM cloaking shells which guides the impinging waves away from the object rendering it invisible.[1,2] Although the proposed methods promise to provide substantial level of invisibility, they all suffer from energy dissipation which makes true invisibility virtually impossible. The goal of our current efforts is to study prospective designs for low loss metamaterials to achieve high levels of electromagnetic invisibility both at the macroscopic and microscopic scales. To achieve this we rely on a mathematical technique called transformational optics that allows the determination of the EMMs that provide a set of desired light paths. Specifically, we study a class of conformal maps that lead to new EMMs that may realize clocking of an object without involvement of magnetism, and concurrently under lower dissipation. These studies will also aid in developing new mathematical and numerical tools for treating electromagnetic interaction with metamaterials both in isotropic and anisotropic regime.

b. Numerical methods in nanoplasmonics: The investigation of the local material response of strongly interactive optical elements requires utilization of highly efficient numerical methods and high performance computing (HPC). As part of this proposal we are developing a parallel finite difference frequency domain (FDFD) codes for calculating the electromagnetic (EM) response of 2D and 3D inhomogeneous systems of random metal-dielectric composites. Additionally, we have been developing a 'memorization' method, an efficient way to do fast searches of conduction paths, providing a solution to the problem in only $O(N^{3/2})$, which is to be compared to $O(N^3)$ for the standard Gauss-Seidel method (N is the number of particles). The numerical codes make possible simulations on the LONI supercomputers of systems with up to 10^6 and 10^4 particles in the 2D and 3D cases, respectively. This allows for a first time to study the local and macroscopic response of real size EM systems including the local response of Active Plasmonics Composite (APC) for solar cell applications (see below), ensembles of particles, including dense semiconductor quantum dots systems, periodic metal particle arrays, photonic nano-circuits and optical switches.

c. Surface Plasma Enhanced Solar Cells (SPESC): The principal objective of this project is to develop a new approach toward inexpensive and highly efficient solar cells based on nano-engineered media. Specifically, a new photo photovoltaic cell is proposed that merges current technology with an Active Plasmonics Composite (APC) to achieve enhanced performance. In recent works, we showed that in the optical and near-IR frequency ranges the radiation reservoir associated with the APC presents drastic departures from any conventional media, resulting in new phenomenon such as enhancement of the spontaneous emission, strong localization of light, and dramatic enhancement of nonlinear optical processes. In this project the enhancement of the SP density of states are utilized to engineer the photovoltaic properties of the SPESC. Substantial improvement of the current yield and conversion efficiencies are expected with the enhanced performance sustained over a broad frequency range. The SPESC design and optimization involves calculation of random systems of up to 1 million strongly interacting particles, thus the utilization of the HPC provided by LONI is crucial. Furthermore, to test the

theoretical predictions we have collaborated with Dr. S. Zivanovic (LA Tech) on a DOE funded project that aims at development/testing of a SPESC prototype.

d. Surface Plasmon based THz transistor: In this project we use surface electromagnetic modes propagating between the interfaces of metal/semiconductors and air to develop an all-optical transistor. Specifically, we rely on a highly doped hetero-junction in connection with optical waveguides to excite and propagate confined SP modes. Two distinct mechanisms, one based on temperature switching and another on charge depletion, will be tested to simulate an effective transistor "I-V" response. Prospective designs have been identified and we are currently at the final stages of this project. The expected outcome is an optoelectronic diode with bandwidth of operation exceeding 1THz. The theoretical results are currently prepared for publication (targeted date Fall 2011) and a prototype will be tested at the Institute for Micromanufacturing.

e. Casimir force reversal in Metamaterials: The Casimir force is a unique phenomenon due to existence of an "infinite ocean" of quantum electromagnetic vacuum fluctuations. For ordinary materials this force is always positive. However, with the invention of the EMMs it may be possible to reverse it sign from attraction to repulsion. In this project we study numerically and analytically the conditions for such reversal to take place. Apart from the fundamental ramification of this project possible applications are envisioned for development of new thin film coatings to address contamination issues in clean rooms, thus lowering the coast of operations and increasing microprocessor chip production efficiency.

f. Continuous Index Photon Traps (CIPT): The optical-mechanical analogy recently demonstrated by Genov *et al.* provides a useful link between the study of light propagation in inhomogeneous media and the motion of massive bodies or light in gravitational potentials[4]. Specifically, we have shown that it possible to directly map in metamaterials the light interaction around gravitational black hole or development novel Photon Traps (CIPTs) as a direct manifestation of a planetary motion, but for light. Our immediate research efforts are focused at improving the existing EMMs designs and establishing collaborations that will allow the experimental validation of the discovered phenomenon.

1. J. B. Pendry, D. Schurig, D. R. Smith, "Controlling Electromagnetic Fields", *Science* 312, 1780 (2006).
2. J. Valentine, S. Zhang, T. Zentgraf, E. Ulin-Avila, D. A Genov, G. Bartal and X. Zhang, "Three Dimensional Optical Metamaterials Exhibiting Negative Refractive Index", *Nature* 455, 376 (2008).
3. D. A. Genov, K. Seal, X. Zhang, V. M. Shalaev, A. K. Sarychev, Z. C. Ying, H. Cao, "Collective Electronic States in Inhomogeneous Media at Critical and Subcritical Metal Concentrations", *Phys. Rev. B* 75, 201403 (2007).
4. D. A. Genov, S. Zhang, X. Zhang, "Mimicking celestial mechanics in metamaterials", *Nature Physics* 5, 687 (2009).

External Funding

- *Artificial optical materials for molding the flow of light*, Louisiana Board of Regents Support Fund – (RCS), PI, recommended for funding ($138,795).
- *Enhancement of the Upper Level Physics Laboratories at Louisiana Tech University*, Louisiana Board of Regents Support Fund, co-PI, approved for funding ($62,943).

Recent Applications for External Funding

- *Electrodeposition of Macroscopic Multilayered Ag/AgO Nanowire Arrays*, NSF – pending funding, co-PI, ($341,441).
- *EDA I6 Challenge: Proposal Narrative for the Louisiana Tech Proof of Concept Center*, Economic Development Administration (EDA), U.S. Department of Commerce (DOC) NSF – pending funding ($1,000,000).

Peer previewed publications and review articles:

- D. A. Genov, R. Oulton, and X. Zhang, "New scaling of light emission in the nanoscale", *Physical Review B,* accepted for publication March 2011.
- D. A. Genov, "General relativity: Optical black-hole analogues", *Nature Photonics* 5, 76-78 (2011)

Invited Seminars:

- "*Redefining the field of Optics with Electromagnetic Metamaterials"*, Department of Applied Physics, Yale University, New Haven, CT, December 8, 2010.
- "*Electromagnetic metamaterials and how to make the Harry Potter invisibility cloak"*, IfM Seminar, Louisiana Tech University, Ruston, LA, March 15, 2011.

Conference Presentations:

- D. A. Genov, S. Zhang, X. Zhang, "Electromagnetic Metamaterials Mimic Celestial Phenomenon in the Lab", *Progress in Electromagnetics Research Symposium* (PIERS)*,* Cambridge, MA, July 5-8 (2010) (Invited talk).
- D. A. Genov, "Molding the Flow of Light with Artificial Optical Materials", *94th OSA Annual Meeting,* Rochester, NY, October 24- 28, (2010). (Invited talk).
- V. Kumaran and D. A. Genov, "Casimir-Polder Force Reversal with air as intermediate medium using Metamaterials", *Louisiana Academy of Sciences 85th Annual Meeting*, Monroe, LA, February 26 (2011). (Best paper award).
- P. C. Mundru and D. A. Genov, "Design of a Generic Cloaking Device", *Louisiana Academy of Sciences 85th Annual Meeting*, Monroe, LA, February 26 (2011).
- Desimone, D. G., M. A. Koorie, A. Thapa, S. R. Animilli, S. Zivanovic, and D. A. Genov, "Theoretical and experimental study of metal-dielectric composite electrodes for polymer solar cell enhancement", *Louisiana Academy of Sciences 85th Annual Meeting*, Monroe, LA, February 26 (2011).
- V. Kumaran and D. A. Genov, "Casimir-Polder Force Reversal using Metamaterials", *77th Annual Meeting of the Southern Section of The American Physical Society,* Baton Rouge, LA, October 20-24 (2010).
- P. C. Mundru and D. A. Genov, "Generic Design of an Invisibility Device", *77th Annual Meeting of the Southern Section of The American Physical Society,* Baton Rouge, LA, October 20-24 (2010).

Teaching at Louisiana Tech University (Fall 2010 - Spring 2011):

PHYS205 (Conceptual Physics I), Fall 2010.
ENGR592/PHYS540/PHYS470s (Computational Methods), Winter 2011.
PHYS202 (Physics for Engineers and Scientists II), Winter 2011.
PHYS522 (Quantum Mechanics), Spring 2011.

Dr. Mark Jarrell, LSU, Computation and Theory of Strongly Correlated Materials

Research Group Members:

M Jarrell, Professor
J. Moreno, Assistant Professor
C. Slezak, Visiting Professor
K.M. Tang, S. Pathak, V. Rousseau, F. Lin, Postdocs
H. Fotso, P. Reis, S. Yang, K. Chen, Kalani Hettiarachchilage, Ricky Nelson, C. Moore, Ch. Ekuma, Sh. Feng, P. Zhang, S. Hall, Graduate Students
David Poliakoff, Joe Caprino, Undergraduate Students
C. Duran, Administrative Assistant

Research Projects

Strongly correlated materials display complex emergent phenomena, or behavior that emerges when many units are assembled that would not be predicted from a complete understanding of the units. This includes transition metal oxides, heavy fermion materials, organic magnets, and spintronic materials. The study of these systems is complicated by the competition of different ground states, including spin, charge and orbital ordering and by the lack of a small parameter. As a result, little progress has been made with conventional theory, and large-scale simulations are needed to form a more complete understanding of models of these systems.

We employ a variety of computational methods to study these systems. The Dynamical Mean Field Approximation (DMFA) and its cluster extensions, including the Dynamical Cluster Approximation (DCA) are at the heart of this approach. These approaches map the lattice onto a cluster embedded in a self-consistently calculated effective medium. Correlations within the cluster are treated explicitly while those at longer length scales are treated in a mean field approximation. The embedded cluster problem is solved using a quantum Monte Carlo (QMC) simulation while disorder can be included by averaging over configurations. Either a perfectly parallel (MPI) or a hybrid parallel (MPI+OpenMP) calculation is used. Nevertheless, the calculation is limited by the amount of memory available on each shared-memory node. A far more significant limitation of this technique is the minus sign problem, which is non-polynomial hard. This means that all simulations of correlated electrons will grow exponentially with the inverse temperature and cluster size making very difficult to treat correlations on the important length scales.

To treat more complex problems a third length scale must be introduced as in the multi-scale many body (MSMB) approach. This is accomplished by a multiple embedding scheme in which correlations over each length scale are treated with an appropriate approximation. Strong correlations at short length scales are treated with an explicit (numerically exact) QMC simulation on a small cluster. This cluster is embedded in the larger cluster where the weaker correlations at intermediate length scales are treated using the parquet approximation which requires both contractions and rotations of rank three tensors (vertices) and a massively parallel computer with at least tens of thousands of processors. This cluster is embedded in an effective medium that is used to treat correlations on the longest length scales.

This year, we dramatically improved the multi-scale formalism, by introducing a dual fermion transformation. The resulting formalism is fully systematic with a small parameter. This paper has been submitted.

Density functional theory is also an essential component of this project. Both the DMFA/DCA and the MSMB approach are parameterized by down folding LDA calculations.

These materials and systems are of great technological importance. Correlated electron materials and especially transition-metal oxides show great promise for novel applications in the semiconductor industry to go beyond CMOS devices for future information processing technologies, which could be

based on “state variables” such as spin. The chapters “Emerging Research Devices” and “Emerging Research Materials” in the 2007 International Technology Roadmap for Semiconductors (ITRS 2007) stress that highly correlated electron systems exhibit coupling between orbital, charge, and spin ordering may enable new devices by greatly enhancing their sensitivity to different applied fields.

We are working in collaboration with Profs. Perdew and Ruzsinszky and their group at Tulane investigating many-body corrections to standard many-body approaches now used in density functional theory, and other ways to look at density functional theory from the many-body perspective. As part of this collaboration, three students from LSU have visited Perdew's group at Tulane and we hold regular meetings, Thursdays at 1:00, via synchronous video.

Our work will lead to a better understanding of these materials, which may lead to better devices based upon them. We also develop and distribute a number of codes that employ architectures at the forefront of computer science, including hyperparallel and multicore machines.

Our work relies upon the large-scale supercomputers available through LONI, the NSF TeraGrid, and the DOE NLCS facilities at ORNL.

We enhance the impact of our work by distributing codes, and related courseware. Two complete courses, Solid State Physics and Classical Electrodynamics are distributed on the group web page, http://www.phys.lsu.edu/~jarrell. In collaboration Prof. Cyrill Slezak, who visits LSU each summer for an extended period, we also participate in Inquiry based RET programs, and we are working with our colleagues to incorporate Inquiry and Active Classroom Teaching techniques into elementary courses in Physics and Astronomy.

As part of our NSF PIRE and LA-SiGMA projects, we teach a complete set of courses in Computational materials Science which are broadcast via interactive synchronous video to all the LA-SiGMA campuses and a number of schools in Germany and Switzerland. Our group is also the lead of a DOE SciDAC project involving researchers at LSU, OSC, UC Davis, and ORNL. The goal of this SciDAC is to develop the MSMB formalism mentioned above.

Recent Publications (submitted, in press, or with a complete reference):

- E. Khatami, K. Mikelsons, D. Galanakis, A. Macridin, J. Moreno, R. T. Scalettar, M. Jarrell Quantum Criticality Due to Incipient Phase Separation in the Two-dimensional Hubbard Model , Phys. Rev. B, **81**, 201101 (2010), arXiv:arXiv:0909.0759.
- V.G. Rousseau, G.G. Batrouni, D.E. Sheehy, J. Moreno, M. Jarrell Pure Mott phases in confined ultra-cold atomic systems , Phys. Rev. Lett., **104**, 051604 (2010), arXiv:arXiv:0909.3543.
- M. Raczkowski, P. Zhang, F. F. Assaad, T. Pruschke, M. Jarrell Phonons and the coherence scale of models of heavy fermions , Phys. Rev. B, **81**, 054444 (2010), arXiv:arXiv:0910.2954.
- Dimitrios Galanakis, Shuxiang Yang, Fakher Assaad, Mark Jarrell, Philip Werner, Matthias Troyer Comment on ``Exact bosonization for an interacting Fermi gas in arbitrary dimensions" , Phys. Rev. Lett. 105, 159701 (2010), arXiv:arXiv:0911.5155.
- Shi-Quan Su, Daniel E. Sheehy, Juana Moreno, Mark Jarrell Dynamical Cluster Quantum Monte Carlo Study of the Single Particle Spectra of Strongly Interacting Fermion Gases , Phys. Rev. A, **81**, 051604 (2010), arXiv:arXiv:0912.3476.
- S. Fuchs, T. Pruschke, M. Jarrell Title: Analytic Continuation of Quantum Monte Carlo Data by Stochastic Analytical Inference , Phys. Rev. E, **81**, 056701, arXiv:arXiv:0912.5204.
- Unjong Yu, Abdol-Madjid Nili, Karlis Mikelsons, Brian Moritz, Juana Moreno, Mark Jarrell Nonlocal effects on magnetism in the diluted magnetic semiconductor $Ga_{1-x}Mn_xAs$, Phys. Rev. Lett., **104**, 037201 (2010), arXiv:arXiv:1001.1716.

- S.-X. Yang, H. Fotso, S.-Q. Su, D. Galanakis, E. Khatami, J.-H. She, J. Moreno, J. Zaanen, and M. Jarrell Proximity of the Superconducting Dome and the Quantum Critical Point in the Two-Dimensional Hubbard Model , Phys. Rev. Lett. 106, 047004 (2011).
- D. Galanakis and E. Khatami and K. Mikelsons and A. Macridin and J. Moreno and D. A. Browne and M. Jarrell Quantum Criticality and Incipient Phase Separation in the Thermodynamic Properties of the Hubbard Model , Philosophical Transactions of the Royal Society A, 369, 1670 (2011).
- V.G. Rousseau and K. Hettiarachchilage and M. Jarrell and J. Moreno Using off-diagonal confinement as a cooling method , submitted for publication.

Recent Presentations and Talks (2010 – 2011)

- *Simulations of Correlated Electrons, What's Under the Superconducting Dome in the Two-Dimensional Hubbard Model?*, presented Feb. 9 as a case study in the *Large Scale Computing and Storage Requirements for Basic Energy Sciences* a BES / ASCR / NERSC Workshop February 9-10, 2010.
- *Quantum Criticality: Key to understanding the Cuprates?*, presented at the third annual all-hands meeting of the LONI Institute, February 10, 2010.
- *Quantum Criticality in the 2-D Hubbard model: what is under the superconducting dome?*, presented as a Condensed Matter Seminar at the National High Magnetic Field Laboratory, February 19, 2010.
- *Quantum Criticality at Finite Doping in the Two Dimensional Hubbard Model* , presented October 27, 2010 at the *ICAM Workshop on Novel Emergent Phenomena Created by Spatial Confinement* October 26-29, 2010.
- *Quantum Criticality at Finite Doping in the Two-Dimensional Hubbard Model* , presented January 7, 2011 at the *PIRE Conference 2011: Petascale Many Body Methods for Complex Correlated Systems* January 7-9, 2011.
- *What's under the superconducting dome in the two-dimensional Hubbard model?* , presented February 21, 2011 as a Physics Department Colloquium at Mississippi State University.
- *Quantum criticality in the Hubbard model*, presented March 25, 2011 as an invited talk at the 2011 March meeting of the American Physical Society.

External Funding:

- *Louisiana Alliance for Simulation-Guided Materials Applications (LA- SiGMA): Leveraging Next Generation Supercomputing for the Study of Complex Multiscale Phenomena in Materials :* EPS-1003897, $20,000,00 ($9,123,947 at LSU) over the five year period, 10/1/10-9/31/15, by the **National Science Foundation, EPSCoR Program**, Investigators: M. Khonsari LA-Regents (PI), M. Jarrell LSU Physics (co-PI), R. Hall LSU Chemistry (co-PI), R. Ramachandran LA Tech Chemistry (co-PI), L. Pratt Tulane Chemical Engineering (co-PI).
- *Simulations of Strongly Correlated Electronic Materials*, DMR-0706379, $375,000 over the three-year period 09/01/07-08/30/11 by the **National Science Foundation, Materials Theory Program**.
- *Graduate Education in Petascale Many Body Methods for Complex Correlated Systems*, OISE-0730290, $2,500,000 over the five-year period 9/1/07-8/31/12 by the **National Science Foundation, Office of International Science and Engineering (OD/OISE)**. Investigators: Juana Moreno (PI) UND, M. Jarrell (Co-PI) and K. Tomko (Co-PI) at the Univ. of Cincinnati.
- *Predictive Capability for Strongly Correlated Systems*, DOE DE-FG02-04ER46129, as part of a Computational Materials Science Network, $121,200 over the three-year period 04/15/07-04/14/10 (to be approved year by year) by the **Department of Energy, Basic Energy Sciences, CMSN** (Warren Pickett, UC Davis, PI).

- Next Generation Multi-Scale Quantum Simulation Software for Strongly Correlated Materials DE-FC02-06ER25792 $3,000,000 over the five-year period 7/06-6/11, by the **Department of Energy, SciDAC**. Investigators: M. Jarrell (PI) and K. Tomko at the Univ. of Cincinnati, Th. Maier (co-PI) and E. DÁzevedo at ORNL, Z. Bai (co-PI) R.T. Scalettar and S. Savrasov at UC Davis.

Recent Applications for External Funding

Proposal	PI Name	Deadline	Amount Requested	Status
36825 - 2	Jin, Rongying	01/13/2011	$4,149,100.00	Submitted
	Sponsor: National Science Foundation - NSF		*Type:* New	
			Date Approved: 01/14/2011	
	Project Title: MIRT: An Integrated Approach to the Discovery of Emergent Quantum Phenomena			
	Proposal Hu, Nai-Wen	*Specialist:Award Specialist:*		
36825 - 1	Chan, Julia Y	09/01/2010	$15,000,000.00	Submitted
	Sponsor: National Science Foundation - NSF		*Type:* Preproposal/NOI	
			Date Approved: 08/31/2010	
	Project Title: CEMRI: LSU Center for Research on Functional Materials (LRFM)			
	Proposal Rhodes, Gretchen Stein	*Specialist:Award Specialist:*		

Dr. Damir Khismatullin, Tulane, Computational modeling and experiments

Research Group Members:

Weixiong Wang, Postdoctoral researcher
Hongzhi Lan, Ph.D. student
Chong Chen, Ph.D. student
Yuan Teng, Masters' student
Theodore Brown, Masters' student

Research Interests

- Cellular biomechanics and adhesion
- Biological transport
- Bubble dynamics and medical ultrasound
- Non-Newtonian fluid mechanics and multiphase flows

Research Projects

I started my appointment as Associate Professor of Biomedical Engineering at Tulane University, with 50% support from the LONI Institute Grant, in August 2008. My research interests focus on understanding the mechanical behavior of biological systems at cellular and tissue levels and the development of novel, optimized approaches for treatment of cardiovascular disease and cancer. Using a combination of state-of-the-art computational models and advanced experimental techniques, my laboratory studies the interactions of blood cells (leukocytes, platelets) and tumor cells with vascular

endothelium under pathophysiological conditions such as inflammation, atherosclerosis, and cancer metastasis. Another aspect of my current research is liver tumor ablation with high-intensity focused ultrasound where my students and I study the mechanical destruction of tumor tissue by ultrasound-produced cavitation bubbles. We also develop novel rheological methods for characterization of living cells and tissues and use our computational models to predict the growth and rupture of intracranial aneurysms. My research is interdisciplinary and involves collaboration with 1) scientists, engineers, and clinicians from leading research institutes and hospitals in Louisiana (Tulane U., LSU Health Sciences Center, Ochsner Medical Center) and other states (Duke U., Boston U., La Jolla Institute for Allergy and Immunology, and Food & Drug Administration); and 2) industry (TA Instruments).

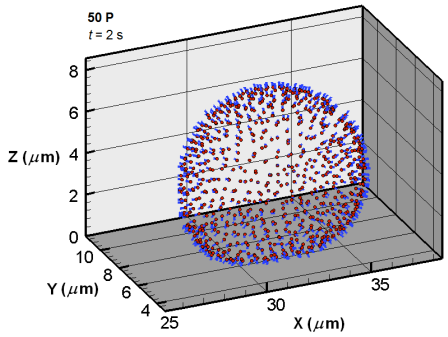

Figure 1: Shape of a rolling white blood cell characterized by cytoplasmic viscosity of 50 P, according to the numerical simulation. The simulation time is 2 s. The wall shear stress is 0.5 dyn/cm2. Red circles are the bases of cell microvilli. Blue lines show the length and orientation of microvilli.

During the fourth year of the grant period (July 2010 - June 2011), we have made the following progress in the four projects of the laboratory.

Project 1: Quantitative Biomechanical Models of Cellular Interactions with Applications in Inflammation, Atherosclerosis, and Thrombosis Since these pathologies are responsible for the majority of death and hospitalization in Louisiana and other states, this project will be of benefit to the majority of Louisiana population. It also helps to establish the strength of the LONI, and Louisiana as a whole, in biomedical computational science.

Computational results:

1. I have completed the development of the fully three-dimensional (3-D) multi-compartmental computational algorithm for rolling and adhesion of deformable cells. This algorithm, shortly abbreviated as VECAM (ViscoElastic Cell Adhesion Model), takes into account the viscoelasticity of the cell cytoplasm and nucleus and model receptor-ligand interactions between the cell and the substrate by probabilistic single-bond kinetics. Using this algorithm, me and Dr. Truskey (Duke U.) have studied the effect of cytoplasmic viscosity on white blood cell (leukocyte) rolling on P-selectin-coated substrate. Our numerical simulation shows that 1) rolling leukocytes deform to a tear-drop shape when the cytoplasmic viscosity is below 300 P (Fig. 1); 2) both the deformation index and the cell-substrate contact area decrease exponentially with the viscosity; 3) an increase in the cell viscosity leads to faster rolling and large variations of instantaneous velocity of the cell (Fig. 2); and 4) there exist a critical value of the cytoplasmic viscosity (500 P) above which leukocytes detach from the substrate even at the wall shear stress of 0.5 dyn/cm2 (Fig. 2). The manuscript with the results of this work has been submitted for publication in Biophysical Journal.

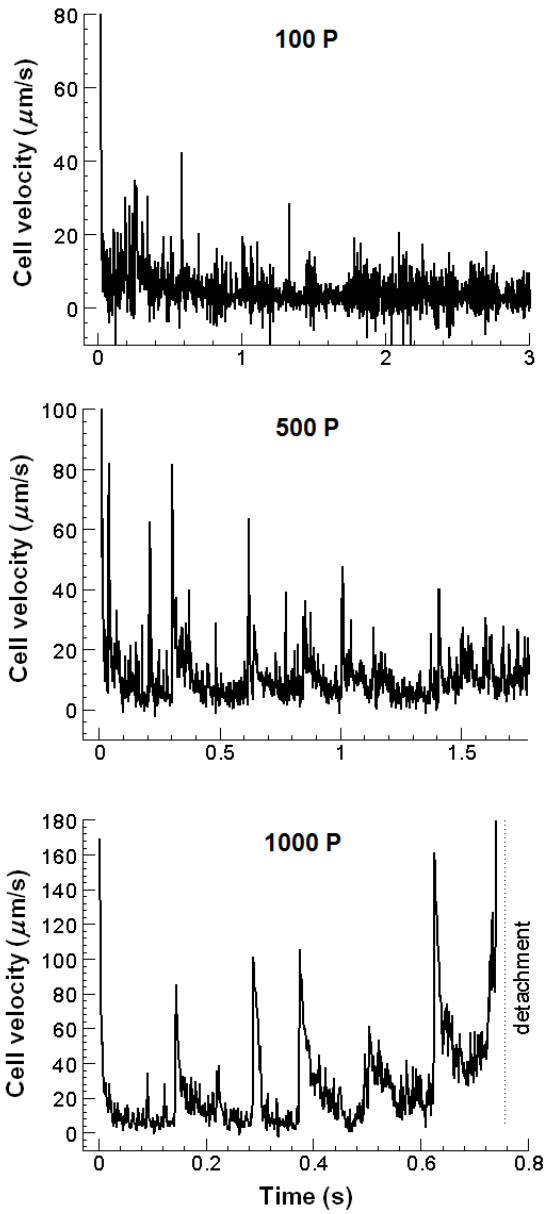

Figure 2: Instantaneous velocity of the rolling white blood cell for different values of the cytoplasmic viscosity.

2. Hongzhi Lan has used the simplified version of my algorithm (without the adhesion subroutine) to investigate the lateral migration of cells and droplets in a microfluidic flow chamber. His analysis indicates that 1) the lateral equilibrium position of oil droplets and leukocytes increases almost linearly with the particle diameter-to-channel height ratio; 2) the equilibrium position and deformation of droplets and cells are highly sensitive to the interfacial/cortical tension; 3) with a higher flow rate, both the deformation index and the orientation angle of deformable particles depend more pronouncedly on the viscosity, which indicate that the mechanical properties of the particles can be efficiently extracted at high flow rates. Overall, these data show that the efficient separation of leukocytes and small oil droplets with low interfacial tension can be achieved in a microfluidic flow chamber provided the channel height is two to 10 times the particle diameter. The results of this study were included in the manuscript submitted for publication in Physics of Fluids.
3. My collaboration with Drs. Cortez and Fauci (Tulane U.) has led to one publication in Physica D in 2011, where we proposed a novel immersed boundary algorithm for the simulation of the shape oscillations of a viscoelastic droplet described by the Oldroyd-B model. Our numerical data are in line with the prediction of small deformation theory.
4. I have received funding from the Louisiana Board of Regents (Research Competitiveness Subprogram) to develop highly efficient parallel algorithms for the simulation of passive and active deformation and adhesion of leukocytes.

The basis of these computational models will be VECAM (which is parallelized using OpenMP directives). My focus will be on mathematical modeling and OpenMP code development, while Hongzhi Lan will develop MPI-PETSc codes.

Experimental results:

1. Chong Chen has studied in vitro the synergistic effect of histamine and TNF-α on rolling and firm adhesion of monocytic cells (THP-1) to confluent layer of endothelial cells (HUVEC) in the Bioflux 200 microfluidic shear flow system (Fluxion Biosciences, CA). Specifically, she grew endothelial cells (passage 3-5) in viewing micro-channels of Bioflux™ 48-well or 24-well plates (Fig. 3); once confluence reached, she activated HUVEC monolayer with histamine, TNF-α, or a combination of these mediators; and finally, she perfused the suspension of monocytic cells through the channels and recorded and analyzed the interactions of these cells with HUVEC. This study shows that when the wall shear stress becomes 1.0 dyn/cm^2 and higher, the flux of slow rolling monocytic cells significantly increases with the co-activation of HUVEC with histamine and TNF-α compared to TNF-α alone activation (Fig. 4). No slow rolling events were observed when HUVEC were stimulated with only histamine. According to flow cytometric analysis, this synergy between histamine and TNF-α is the result of the upregulation of the endothelial surface expression of all four major cell adhesion molecules (P-selectin, E-selectin, VCAM-1, and ICAM-1) for monocytes. The manuscript with the results of this work has been submitted for publication in the Journal of Immunology.

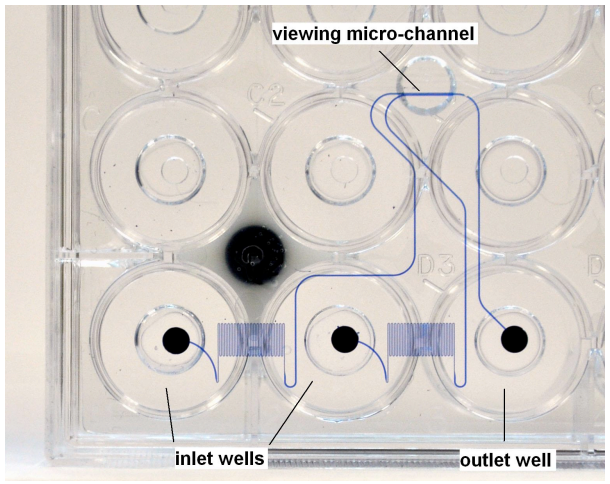

Figure 3: Photograph of a Bioflux™ 24-well plate showing micro-channels that connect two inlet wells and one outlet well.

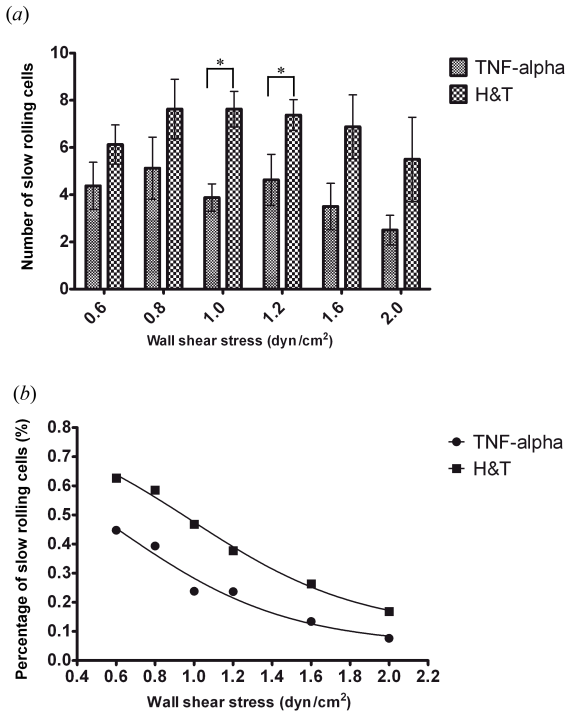

Figure 4: (a) Number and (b) percentage of slow rolling cells on TNF-α- and histamine + TNF-α-activated HUVEC as a function of the wall shear stress. The image area is 937×700 μm^2. *p < 0.05.

2. Teddy Brown has developed a cell-free system for platelet aggregation and thrombus formation. The essence of this system is fluorescent carboxylate microspheres coated with recombinant human GPIb-α (platelet glycoprotein). Using this system, he showed that histamine upregulates platelet adhesion on HUVEC. We hypothesize that histamine increases adhesion of platelets because of the release of vWF and associated P-selectin from the Weibel-Palade bodies of endothelial cells. To test this hypothesis, Teddy is conducting

ELISA tests and flow cytometry. He also does experiments with human platelets to validate our cell-free system. His work will be presented at the 2011 BMES meeting and we are preparing a manuscript that will be submitted to Annals of Biomedical Engineering.

Project 2: Development of Novel Methods for Rheological Characterization of Biological Materials

1. Dr. Weixiong Wang, Dr. De Kee (Tulane U.) and me have numerically analyzed wall slip, secondary flow, and end effects in rheological measurements of non-Newtonian fluids in a double concentric cylinder rheometer and a vane rheometer. This study has resulted into two papers published in the Journal of Rheology in 2010 and the Journal of non-Newtonian Fluid Mechanics in 2011, respectively. In the former paper, we showed that a double concentric cylinder rheometer equipped with a slotted rotor can measure the fluid properties with enhanced accuracy and less sensitivity to the wall slip velocity that a rheometer with a non-slotted rotor. In the latter paper, we showed that the double concentric cylinder rheometer with slotted rotor (DCCR/SR) is able to accurately measure rheological properties of a wider spectrum of test fluids than a vane rheometer because of significant reduction of the end and secondary flow effects.
2. Dr. Weixiong Wang, Dr. De Kee (Tulane U.) and me have also developed the numerical model of the slotted plate technique for yield stress measurement. Using this model, we studied the effects of the plate geometry (including the shape of the plate edges and the number and area of slots) on the accuracy of this rheological method. Our recommendations for the optimal design is a thin plate with sharp from and rear edges, more than 12 slots, and the slot area ratio of more than 80%. The manuscript with the results of this work has been submitted for publication in Rheologica Acta.
3. Yuan Teng continues her microrheological analysis of various polymer and biological solutions. In 2010-2011, her focus was on the characterization of dextran, agarose, and Xantham gum solutions by multiple particle-tracking microrheology using our deterministic motion cancellation algorithm and validation of the data via measurement with a standard rheometer. It is anticipated that she will submit her first paper in summer 2011.

Project 3: Numerical Study of Blood Flow in Cerebral Vessels with Aneurysm and in Capillary Sprouts Our aneurysm research is highly transformative and extremely important because it will lead to new strategies for surgical treatment of intracranial aneurysms that will increase the survival rate of the patients after surgery.

1. Dr. Weixiong Wang and me, in collaboration with Dr. Arthur Ulm (LSU Health Sciences Center) and his residents, and Dr. De Kee (Tulane U.), have worked in 2010-2011 on the development of the anatomically correct model of blood flow in a giant cerebral aneurysm (Fig. 5). With this model, we have investigated the aneurysm embolization with a yield stress fluid material. Our results show that 1) aneurysm embolization requires the yield stress values of higher than 20 Pa; 2) yield stress fluid treatment can substantially reduce flow recirculation in the aneurysm and the size of the inflow jet impingement zone and the effect of this treatment is stronger than that can be achieved by coil treatment. The manuscript with the results of this work has been submitted to the Journal of Biomechanical Engineering.

2. In collaboration with Dr. Murfee (Tulane U.), Dr. Weixiong and me have developed the computational model for blood flow in permeable and impermeable capillary sprouts. This model was used to determine the distribution of fluid shear stresses in sprouts under different flow conditions and sprout geometries. The paper with the results of this work has been published in Cardiovascular Engineering and Technology in 2011.

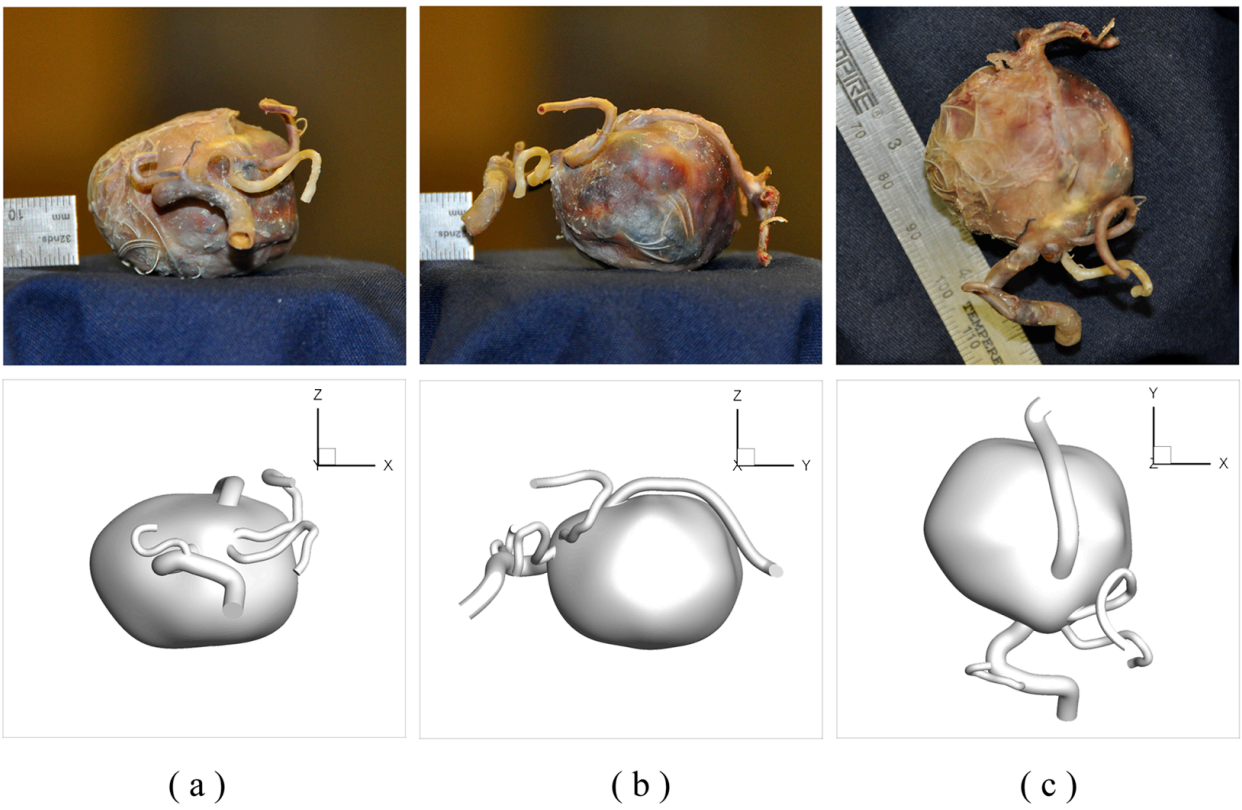

Figure 5: Reconstruction of the model geometry from a postmortem aneurysm specimen. Top: photographs of the aneurysm taken from (a) front, (b) right, and (c) top views. Bottom: the shape of the model aneurysm from (a) front, (b) right, and (c) top views.

Project 4: Liver tumor ablation by combination of percutaneous ethanol injection and high-intensity focused ultrasound This is a highly transformative and extremely important project because it will result in a novel and optimized method for ablation of large and metastatic tumor masses in the liver. It should be noted that primary liver cancer (i.e., hepatocellular carcinoma) is the third common cause of cancer-related deaths in the world and its incidence rate in the United States increases every year due to the spread of hepatitis B and C viral infections. The high mortality rate of hepatocellular carcinoma can be explained by the fact that this disease has little or no symptoms when tumor mass is small, leading to a large

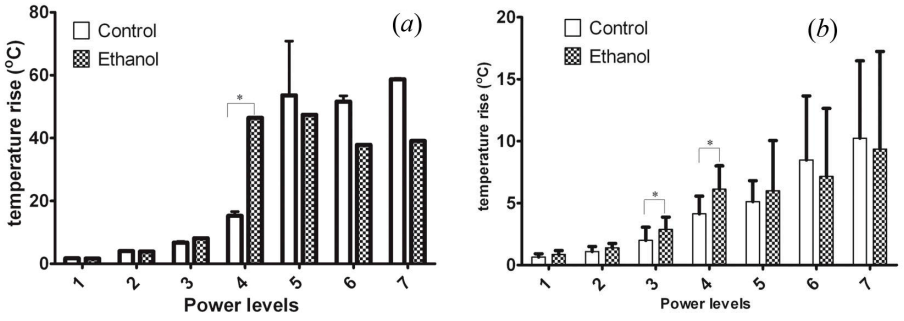

Figure 6: (a) TMM and (b) bovine liver tissue heating by HIFU and PEI at different values of the acoustic power. Level 1: 1.3 W, level 2: 3.2 W, level 3: 5.0 W, level 4: 13.0 W, level 5: 16.2 W, level 6: 20.9 W, and level 7: 26.8 W. * indicates the significance level $p < 0.05$.

number of patients with advanced disease. Our project targets this group of patients.
Chong Chen together with Dr. Myers' laboratory (FDA) and me have investigated the cavitation activity and temperature rise in a hydrogel-based TMM phantom and excised bovine liver treated with ethanol and insonated with a 0.825 MHz focused acoustic transducer. Cavitation events were quantified by three independent techniques: B-mode ultrasound imaging, needle hydrophone measurements, and passive cavitation detection. Temperature in or near the focal zone was measured by thermocouples embedded in the samples. The results of this study indicate that the treatment of tissue phantom and bovine liver with ethanol reduces their threshold pressure for inertial cavitation. This in turn leads to a sudden rise in temperature in ethanol-treated samples at a lower acoustic power than that in untreated ones (Fig. 6). The analysis of passive cavitation detection data shows that once the threshold acoustic power is reached, inertial cavitation becomes a major contributor to acoustic scattering in ethanol-treated phantoms and bovine liver samples. The manuscript with the results of this work was submitted for publication in Ultrasound in Medicine and Biology.

Publications

- H. Lan and D.B. Khismatullin, "Three-dimensional numerical simulation of the lateral migration of oil droplets and leukocytes in rectangular microchannels," *Phys. Fluids* (2011, submitted).
- W. Wang, F. Graziano, V. Russo, Arthur J. Ulm, D. De Kee, and D.B. Khismatullin, "Giant intracranial aneurysm embolization with a yield stress fluid material: Insights from CFD analysis," *J. Biomech. Eng.* (2011, submitted).
- C. Chen, Y. Liu, S. Maruvada, M. Myers, and D.B. Khismatullin, "Effect of ethanol injection on cavitation and heating of tissues exposed to high intensity focused ultrasound," *Ultrasound Med. Biol.* (2011, submitted).
- C. Chen and D.B. Khismatullin, "In vitro study predicts the synergistic effect of histamine and TNF-alpha on monocyte-endothelial cell interactions" *J. Immunol.* (2011, submitted).
- W. Wang, B. Meng, D. De Kee, and D.B. Khismatullin, "Optimization of a slotted plate device for low yield stress measurements," *Rheol. Acta* (2011, submitted).
- D.B. Khismatullin and G.A. Truskey, "Leukocyte rolling on P-selectin: A 3D numerical study of the effect of cytoplasmic viscosity," *Biophys. J.* (2011, submitted).
- J.C. Chrispell, R. Cortez, D.B. Khismatullin, and L.J. Fauci, "Shape oscillations of a droplet in an Oldroyd-B fluid," *Physica D* (2011, **in press**)
- W. Wang, D. De Kee, and D.B. Khismatullin, "Numerical simulation of power law and yield stress fluid flows in double concentric cylinder with slotted rotor and vane geometries" *J. Non-Newtonian Fluid Mech.* **166**, 734-744 (2011).
- P. C. Stapor, W. Wang, W. L. Murfee, and D.B. Khismatullin, "The distribution of fluid shear stresses in capillary sprouts" *Cardiovas. Eng. Tech.* **2**, 124-136 (2011).
- W. Wang, H. Zhu, D. De Kee, and D.B. Khismatullin, "Numerical investigation of the reduction of wall slip effects for yield stress fluids in a double concentric cylinder rheometer with slotted rotor" *J. Rheol.* **54**, 1267-1283 (2010).

Presentations

- W. Wang, B. Meng, D. Rice, D. Khismatullin, and D. De Kee, "Slotted plate device for low yield stress measurements," Canadian Society of Rheology Meeting, June 6-7, 2011 — Montreal, Canada.
- Y. Teng, W. Wang, and D.B. Khismatullin, "Development of multiple-particle-tracking microrheology for fluids experiencing deterministic motion," 82nd Annual Meeting of the Society of Rheology, October 24-28, 2010 — Santa Fe, New Mexico.

- W. Wang, D.B. Khismatullin, H. Zhu, and D. De Kee, "Numerical analysis of double concentric cylinder rheometer with slotted rotor," 82nd Annual Meeting of the Society of Rheology, October 24-28, 2010 — Santa Fe, New Mexico.
- C. Chen and D.B. Khismatullin, "Histamine induces monocyte interactions with arterial endothelium in vitro," 2010 BMES Annual Fall Meeting, October 6-9, 2010 — Austin, Texas.
- W. Wang, F. Graziano, V. Russo, and D.B. Khismatullin, "Numerical study of blood flow after embolization of cerebral aneurysm with yield stress fluids," 2010 BMES Annual Fall Meeting, October 6-9, 2010 — Austin, Texas.
- W. Wang, P. C. Stapor, W.L. Murfee, and D.B. Khismatullin, "Influence of permeability on shear stress distribution along capillary sprouts," 2010 BMES Annual Fall Meeting, October 6-9, 2010 — Austin, Texas.
- H. Lan and D.B. Khismatullin, "3-D numerical simulation of lateral migration of cells and deformable particles in shear flow," 2010 BMES Annual Fall Meeting, October 6-9, 2010 — Austin, Texas.
- D.B. Khismatullin, M. Pospieszalska, and K. Ley, "Influence of cell deformation, tether formation and catch/slip bond behavior on leukocyte rolling," 2010 BMES Annual Fall Meeting, October 6-9, 2010 — Austin, Texas.

External Funding

- Louisiana Board of Regents, Research Competitiveness Subprogram (BoR-RCS). Title: *Parallel algorithms for the simulation of cellular deformation and adhesion*. Role: Principal Investigator. Funding amount: $148,089 (total costs) for 06/01/2011 – 05/31/2014.

Dr. David L. Mobley, UNO, Computational Free Energy Studies from Molecular Simulations

Research Group Members:

Pavel Klimovich (graduate student), Anasuya Kolavennu (graduate student), Jessica Fuselier (graduate student, Physics), Shuai Liu (graduate student), Christopher Savoie (finishing undergraduate student), and summer students (undergraduate students Vivian Jaber and Emily Taylor (Chemical Engineering, Manhattan College, New York), as well as Brandon Edwards, a school teacher from Washington, DC). The preceding are all UNO Chemistry students except otherwise noted. Also, I jointly supervise Gabriel Rocklin (a graduate student at the University of California, San Francisco) together with Ken Dill and Brian Shoichet (both at UCSF).

Research Interests

Our group specializes in computational studies at the interface of chemistry, physics, and biology, and a particular emphasis is problems relating to drug discovery. We focus on applying molecular simulations to compute thermodynamic properties relating to protein-ligand interactions and solubility. This work is designed to impact the pharmaceutical drug discovery process, providing tools to make it substantially easier to develop new drugs.

Research Projects

My research group focuses on understanding, predicting, and manipulating free energies. These govern a huge array of interesting physical processes, driving biomolecular association and dissociation, solubility, permeation, and transfer between different environments. We develop and apply computational methods to predict binding free energies, transfer free energies, and solubilities based on computer simulations of the molecules involved.

Solubilities, transfer free energies, and binding free energies are all key components of the pharmaceutical drug discovery process. Today, the drug discovery process involves much expensive and time-consuming trial-and-error. We seek to develop and advance methods that can be used directly in pharmaceutical discovery to predict, based on structure, which molecules will bind sufficiently well to a target protein to make a good drug, and how to optimize these molecules to achieve adequate solubility to function as a pharmaceutical drug.

Our work on binding free energies between proteins and small-molecule ligands was essentially the first work to compute rigorous binding free energies between proteins and small molecule ligands, without requiring the bound structure of the protein and ligand as input. Using molecular dynamics simulations, we computed binding free energies beginning from the unbound protein structure, and predicted ligand binding modes. We successfully tested the approach we developed for making blind predictions two different model binding sites. Current work includes working in collaboration with Vertex Pharmaceuticals to better understand and more accurately model potential inhibitors of DNA gyrase to aid in development of new antibacterials. We are also studying BIR3 XIAP, an anti-cancer target, in an effort to guide discovery of new inhibitors. Also, in collaboration with Grover Waldrop (experimental biology, LSU) we are working to find new potential anti-tuberculosis drugs targeting biotin carboxylase. Ultimately, the methods we are developing for studying protein-ligand binding free energies will have application to computational drug discovery, biomolecular association generally, and to guide design of new enzymes.

Because of most biomolecular interactions take place in an aqueous environment, we also have a particular interest in assessing the accuracy of our models for describing molecular interactions with water. This has led to a focus on hydration (gas-to-water transfer) free energies, and we have several publications in this area. We have largely been fairly successful in predicting solvation free energies, though failures have also guided us to deficiencies in the force field and point the way towards further force field developments. Consequently, this work has the potential for large payoffs in diverse areas, from protein-ligand binding, to protein folding and protein structure prediction, to understanding surface interactions and properties of materials.

A more recent focus in the group is predicting solubilities of small molecules – the concentration above which a molecule will fail to dissolve in water. This is important in a huge number of contexts, from oil extraction (where pipelines can be blocked by solid deposits) to drug discovery (where most drugs must dissolve after being taken in pill form). Solubility is simple in theory – it is determined by the balance of favorable interactions within a solid form, with favorable interactions between the molecule and water. But this is easier said than predicted, and computational methods are only just reaching the point where this is becoming a tractable problem. Given our expertise in solvation, we have a handle on half of the solubility problem, and are now beginning work to handle the solid state, in collaboration with a group from the University of Notre Dame. Improved methods for predicting solubilities will help guide efforts to control solubility, for example in a drug discovery or chemical reaction context.

Overall, the research has the potential to transform a variety of fields that are currently governed by experimental trial and error. Computational methods have so far been unreliable enough for these problems that it is typically preferred to simply do the experiment. This research will help bring computation to the point where computational results can reliably predict experiments, paving the way for computers to guide scientific discovery rather than trial and error. Experiment could be used to confirm computational predictions, rather than the current approach of merely using computation to help rationalize experimental results.

This work is heavily dependent on existing Louisiana cyberinfrastructure, in particular the Louisiana Optical Network Initiative (LONI). It is tremendously demanding computationally, and so high performance computing is key to pushing these models forwards.

Much of my work is collaborative. I have active collaborations with experimental with experimental groups at Louisiana State University (including Grover Waldrop and Fareed Aboul-Ela) and pharmaceutical companies including Vertex Pharmaceuticals (Boston, MA). I already have existing collaborations with an experimental group at the University of California, San Francisco (UCSF), and other computational groups at UCSF, Merck, the University of Notre Dame, and others. The work enhances the research infrastructure of the state by making the potential for absolute binding free energy calculations -- something done only a few places in the world -- available to potential collaborators, both in academia and industry, in the state. Long-term, a goal is that this work may make Louisiana more attractive to pharmaceutical companies.

I handle graduate recruiting and selections for the Chemistry department, so there are a variety of outreach activities associated with that. Additionally, this summer I am hosting two full-time undergraduate students (one on an REU) and an RET student.

Publications

- J. D. Chodera*, **D. L. Mobley**, M. R. Shirts, R. W. Dixon, K. Branson, V. S. Pande, "Alchemical free energy methods for drug discovery: Progress and challenges," *Current Opinion in Structural Biology* (2010).
- X. Gu, S. Izenwasser, D. Wade, A. Housman, G. Gulasey, J. B. Rhoden, C. D. Savoie, **D. L. Mobley**, S. A. Lomenzo, and M. D. Trudell*. "Synthesis and Structure-Activity Studies of Benzyl Ester Meperidine and Normeperidine Derivatives as Selective Serotonin Transporter Ligands", *Bioorg. Med. Chem. Lett.* **18**: 8356-8364, 2010.
- P. V. Klimovich and **D. L. Mobley***, "Predicting hydration free energies using all-atom molecular dynamics simulations and multiple starting conformations", J. Computer-Aided Molecular Design **24**: 307-316 (2010).

Presentations and Talks

- "Insights into solvent effects from free energy calculations", joint Southwest/Southeast Meeting of the American Chemical Society, New Orleans, LA, Dec. 1, 2010. Invited talk.
- "Predicting Protein-ligand Binding Affinities from Molecular Simulations", BioMaPS Institute, Rutgers University, October 5, 2010. Invited talk.
- "Challenges in predicting binding free energies", CECAM Meeting on Dynamics and Thermodynamics of Biomolecular Interactions, Palaiseau, France, May 2011. Invited talk.

External Funding (proposed, pending, awarded)

Pending:

"Improving alchemical methods for predicting protein-ligand binding", NIH R-15 grant, Feb. 25, 2011. $351,840. As PI.

Dr. Zhenyu Ouyang, SUBR,

Research Group Members:

Mr. Gefu Ji, Ph.D. Student
Mr. Jay Kumar Perneedi, Master Student
Mr. Vijay Morampudi, Master Student
Mr. Raghvan Madawela, Master Student

Research Interests

- Fracture mechanics and fatigue of composite materials and structures;
- Adhesively bonded joints in composite structures;
- Self-adaptive, self-monitoring, and self-healing multi-functional materials and structures;
- Lightweight composite materials and structures with superior impact mitigation capability;
- Local fracture characterization of advanced materials and structures.

Areas of Future Research

- Multi-functional materials for innovative aerospace materials & structures;
- Bio-mimic or/and bio-inspired functionally graded hybrid materials and structures for the next generation aerospace structures, featured by reliability, intelligence, and environment friendliness;
- Multi-physical modeling of multifunctional aerospace materials and structures within the framework of multi-scale modeling (from macro-level to meso-level, and then down to molecular level) for composite structures by combining Molecular Dynamics (MD) simulation, Cohesive Zone Model and Extended Finite Element Method (XFEM).

Publications Published Or Accepted

- **Zhenyu Ouyang**, Gefu Ji and Guoqiang Li, 2010, On Approximately Realizing and Characterizing Pure Mode-I Interface Fracture between Bonded Dissimilar Materials, *ASME Journal of Applied Mechanics*, vol. 78 (3), p. 031020.
- Gefu Ji, **Zhenyu Ouyang** and Guoqiang Li, Local Interface Shear Fracture of Bonded Steel Joints with Various Bondline Thicknesses, *Experimental Mechanics*, DOI: 10.1007/s11340-011-9507-y (online first).
- Gefu Ji, **Zhenyu Ouyang** and Guoqiang Li, 2011, Effects of Bondline Thickness on Mode-II Interfacial Laws of Bonded Laminated Composite Plate, *International Journal of Fracture*, vol. 168(2), pp. 197-207.
- Gefu Ji, **Zhenyu Ouyang**, Guoqiang Li, Samuel Ibekwe and Su-Seng Pang, Healable and Repeatable Adhesively Bonded Joint, *ASME* 2011 *Pressure Vessels & Piping Conference*, July 17-21, 2011, Baltimore, Maryland, USA.
- Gefu Ji, **Zhenyu Ouyang**, Guoqiang Li, Wei Xu, Dwayne Jerro, and Su-Seng Pang, Effects of Adhesive Thickness on Global and Local Mixed Mode I/II Interfacial Fracture of Bonded Steel Joints, *ASME* 2011 *Pressure Vessels & Piping Conference*, July 17-21, 2011, Baltimore, Maryland, USA.
- Raghvan Madawela, **Zhenyu Ouyang**, Gefu Ji, Guoqiang Li and Samuel Ibekwe, Mechanical Properties of New Hybrid Materials: Metallic Foam Filled with Syntactic Foam, *ASME* 2011 *Pressure Vessels & Piping Conference*, July 17-21, 2011, Baltimore, Maryland, USA.
- Morampudi Vijay, **Zhenyu Ouyang**, Gefu Ji, Guoqiang Li and Dwayne Jerro, Characterization of Short Basalt Fiber Reinforced Syntactic Foams, *ASME* 2011 *Pressure Vessels & Piping Conference*, July 17-21, 2011, Baltimore, Maryland, USA.

Publication Under Review

- Gefu Ji, **Zhenyu Ouyang**, and Guoqiang Li, Impact/Debonding Tolerant Sandwich Panel with Novel Hybrid Foam Core, *Composite Science and Technology* (under review).
- Gefu Ji, Guoqiang Li, and **Zhenyu Ouyang**, Local Interface Fracture of Healable and Repeatable Adhesive Bonded Joint, *Composite Science and Technology* (under review).
- Gefu Ji, **Zhenyu Ouyang**, and Guoqiang Li, Effects of Adhesive Thickness on Global and Local Mixed Mode I/II Interfacial Fracture of Bonded Steel Joints, *International Journal of Adhesion and Adhesives* (under review).

Publication Under Development

- Raghvan Madawela, **Zhenyu Ouyang**, Guoqiang Li, and Gefu Ji, Physical Properties of New Hybrid Materials: Metallic Foam Filled with Syntactic Foam, *Composites Science and Technology* (to be submitted).
- Vijay Morampudi, **Zhenyu Ouyang**, Guoqiang Li, and Gefu Ji, Static and Dynamic Test of Short Basalt Fiber Reinforced Syntactic Foams, *Composite B* (to be submitted).
- **Zhenyu Ouyang**, Gefu Ji, Guoqiang Li, Novel Metallic Foam Based Grid Structure, *International Journal of Solids and Structures* (to be submitted).

External Funding

- Negative Poisson's Ratio and SMA Based Metallic Foam Reinforced Adhesive Layer in Bonded Joints for Aerospace Structures funded by Louisianan Space Consortium (LaSPACE), PI: G. Li, Co-PI: **Zhenyu Ouyang**, 12/01/10-11/31/11, $750,000.
- An Integrated Topology and Multi-Scale Optimization of Protective Structures" funded by Army Research Office, PI: G. Li, Co-PI: **Zhenyu Ouyang**, 07/01/09-06/30/12, $120,000.
- A Shape Memory Polymer Based Self-Healing Sealant for Expansion Joint", Transportation Research Board (TRB) of the National Research Council (NRC) and Louisiana Transportation Research Center (LTRC), PI: Guoqiang Li (PI), Co-PI: **Zhenyu Ouyang**, $135,000 (TRB) and $29,000 (LTRC matching); (3/1/2009–09/31/2012).

Recent Applications for External Funding

- Manufacturing, Characterization and Optimization of Functionally Graded and Nanophased Hybrid Sandwich Core, 10/01/2011-09/31/2014, $317,943, National Science Foundation, **PI: Dr. Zhenyu Ouyang**, co-PI: Dr. Guoqiang Li.
- Bio-inspired Shape Memory Polymer Fiber Reinforced Thermosetting Polymer Composite for Self-healing
- Structural-length Scale Damage, 12/01/2011-11/30/2014, $417,943, US ARMY RESEARCH, HBCU/MSI, DoD, PI: Dr. Guoqiang Li, co-PI: Dr. **Zhenyu Ouyang** and Dr. Samuel Ibekwe.
- Bio-mimetic Self-healing Composite Sandwich for Impact Tolerant NextGen Aerospace Structures, 10/01/2011-9/30/2014, $1,410,000, NASA/ EPSCoR, PI: Dr. Guoqiang Li, Subcontract-PI: Dr. **Zhenyu Ouyang**, Co-PI: Dr. Samuel Ibekwe, Dr. Su-Seng Pang, and Dr. Donghui Zhang.

Recent Applications for External Funding - Declined

- Advanced Sandwich Panel with Metallic Foam Based Grid and SMA Composite Skin for Impact Mitigation, 06/01/2010-05/31/2013, $118,751 for three years, Board Regent of Louisiana, **PI: Dr. Zhenyu Ouyang**, co-PI: Dr. Guoqiang Li.
- Novel Open-cell Metallic Foam Based Multi-functional Composite Decks for Highway Bridges, 12/01/2010-11/31/2013, $250,000 for three years, U.S. Department of Transportation, Federal Highway Administration, PI: Dr. **Zhenyu Ouyang**.

- Smart Joint Bonded by Adhesive with Negative Poisson's Ratio and Shape Memory Capability, 07/01/2011-06/31/2014, $317,943 for three years, National Science Foundation, **PI: Dr. Zhenyu Ouyang**, co-PI: Dr. Guoqiang Li.

Teaching at SUBR (Fall 2010 - Spring 2011):
ENGR 120, Introduction to Engineering, Undergraduate Level
MEEN 336, Composite Materials, Undergraduate Level
ENGR 551, Fracture Mechanics and Fatigue, Graduate Level
MEEN 563, Composite Materials, Graduate Level

Dr. Caz Taylor, Tulane, Population dynamics and connectivity of Blue Crabs

Research Group Members:
Erin Grey, Postdoctoral researcher
Hideki Fujioka. LI Computational scientist
Woody Nero, NOAA. Particle tracking model for brown shrimp
Dong Ko, Naval Research Lab. Ocean circulation model
Harriet Perry, Director of GCRL, USM. Blue crab biology and identification of plankton
Michael Bartlein, Undergraduate (summer intern)
Other Undergraduate field assistants: Shae Crain, Kyle Coblentz, Susan Chaisson, Benjamin Jones

Research Project
Blue Crabs are one of the most important species in the Gulf of Mexico from commercial and ecological perspectives. This key species was just beginning its spawning season when the Deepwater Horizon oil spill occurred. We are undertaking intensive sampling of larval blue crabs both in the ocean via plankton tows and in estuaries where the juvenile crabs settle. Using a particle-tracking approach in concert with a fine-scale, spatially explicit ocean circulation model, we will estimate connectivity of the blue crab population in estuaries of the Gulf of Mexico and incorporate outputs of lethal and sublethal effects of oil and dispersants on larvae. The particle-tracking model will build in the extent and concentration of the oil spill on blue crab dispersal and recruitment. Interdisciplinary research opportunities will be provided to undergraduate and graduate students. The commercial importance of the blue crab fishery in the Gulf accentuates the broad societal impact of this project. There are tremendous resources at risk in the Gulf of Mexico as a result of the Deepwater Horizon oil spill and this study will supply critical information about effects on the environment.

***Status*:** Woody Nero has developed a version of the particle tracking model written in matlab using obtained ocean circulation data from a model developed by Dong Ko for 2007, 2008, 2009, and 2010 (~2 TB). Hideki rewrote the model in C++ and it is now running on a Mac Pro in my lab. Hideki worked on a parallel implementation of the code for LONI. We have not yet addressed the data storage issues that we will need to address to run this model on LONI.

In the last year, a computational undergraduate student, Michael Bartlein (physics major at Tulane), funded in summer 2010 by an internship from the Center for Computational Science (CCS) and in fall by a NSF RAPID grant and in Spring by a grant from the Tulane provost's office has been working in my lab. Michael has redesigned the C++ code to make it more modular and flexible and has been conducting research by simulating different scenarios of larval dispersal.

Last summer, funded by a NSF RAPID grant to address the DWH oil spill, we conducted field sampling to gather data with which to validate the model. We collected a large number of megalopal stage crabs at 9 sites along the coast from Appalachicola, FL to Galveston, TX and also conducted plankton tows to

sample larval stages of crabs. Samples are still being processed. In 2011, we will repeat the field sampling at 4 sites funded by an award ($20,000) from the Center for Bioenvironmental Research at Tulane/Xavier.

Presentations/Talks

- Taylor and Grey. Population dynamics of Blue crabs. Invited Seminar, University of Georgia Feb 2011
- Taylor and Grey. The impacts of Deepwater Horizon oil spill on blue crabs. Invited Seminar, Loyola University Nov 2010
- Taylor. Oil Spill Research Conference (invited panelist) November 2010
- Taylor. The impacts of Deepwater Horizon oil spill on blue crabs. Conference talk *e-hormone*, New Orleans, October 2010
- Grey and Taylor. The impacts of the DWH oil spill on recruitment of blue crabs. Conference talk. *Benthic Ecology*. Mobile, AL. Feb 2011
- Grey and Taylor. The impacts of the DWH oil spill on recruitment of blue crabs. Conference talk. *Geological Society of America*. New Orleans, LA March 2011

External Funding Awarded

NSF 6/1/10-5/31/11. RAPID Deepwater Horizon oil spill: Impacts on Blue Crab population dynamics and connectivity. $200k

External Funding Pending

NSF 6/1/10-5/31/11. Connectivity and metapopulation dynamics of Blue Crabs in the Gulf of Mexico. $555k

Christopher Taylor, UNO,

Research Group Members:

Jonathan Brown, Undergraduate Student
Joseph Coco, Masters Student
A. Murat Eren, PhD Student
Mohamad Qayoom, PhD Student
Qi Zhang, PhD Student

Research Projects

Dr. Christopher Taylor is an assistant professor in the Department of Computer Science at the University of New Orleans. He is a member of the bioinformatics group and has a joint appointment at the Research Institute for Children (RIC), part of the Children's Hospital of New Orleans. RIC provides Dr. Taylor with research support and collaborative opportunities with a staff of LSU-HSC faculty performing research at the institute. Dr. Taylor's research is highly collaborative in nature and he works with a variety of biologist to design algorithms for analysis of experimental data. In particular his group focuses on:

- Analysis and Visualization of Human Microbiome Data
    - Classification of diverse constituents present in samples
    - Visualization of bacterial community composition
    - New methods of sequence classification
- High-throughput Sequence Mapping and Databasing
    - Mapping sequencing reads to various genomes
    - Storage and retrieval of sequencing data

- Analysis and Visualization of RNA Sequencing Data
    - Discovery of exogenous agents in RNA-Seq data
    - Assembly of transcripts and reclassification

High-throughput sequencing and DNA Microarray technologies have transformed the landscape of research in biology from the single experiment-single result model to an interrogation of the entire genome from a single experiment. These technologies provide researchers with an abundance of data, but also necessitate the development of specialized analysis algorithms to process the results. Many of the emerging technologies are rapidly changing and present new computational challenges with each new generation of equipment. Our research group collaborates closely with the biologists who perform these experiments to develop new algorithms and analysis techniques to tackle these constantly evolving problems.

One of our recent collaborations involves researchers at Tulane Health Sciences Center and Xavier University. This work was funded by the NIH to study the effects of MicroRNAs transfected into cells. High-throughput sequencing technology is being used for RNA-Sequencing to interrogate on a genomic scale and we are helping to design algorithms to analyze this data. Both Mohamad Qayoom and Qi Zhang are involved in this project. We are working to map the RNA-Seq data back to the human genome and analyze expression levels that are modulated by microRNAs. This involves mapping reads that span exon junctions and calculating relative abundance of transcripts across samples. We are also looking for exogenous DNA by mapping the reads that don't map back to the human genome to other organisms and databases. Visualization for this data has been developed by Joseph Coco who recently graduated with a Master's degree based on this work.

Our research group is also collaborating with a microbiologist at Children's Hospital who is affiliated with LSU-HSC. We are studying the Human microbiome to assess the effects of the colonization of bacteria that lives on and inside of the human body. This work requires development of algorithms to interpret sequencing data and downstream analysis of the results. Murat Eren has developed a framework for this analysis that is easily usable by our collaborators with minimal computing knowledge. This framework is highly scalable and will be interfaced with distributed computing resources in future work to allow for faster and more accurate analysis. The framework provides visualization of the data submitted by the biologist in the form of pie charts, clustering heatmaps, and rarefaction curves. Murat recently graduated with a PhD based on this work.

Finally, our group has also performed preliminary work on analyzing mutation rates using high-throughput sequencing data. This is a burgeoning collaboration with another researcher at LSU-HSC and Children's Hospital to investigate the importance of specific mutations in immune response pathways. This work involves custom software development for analysis of pairwise sequence alignments in addition to development of strategies for efficient sequence mapping and analysis.

Publications

Invited Book Chapters:

- Neerja Karnani, Christopher M. Taylor and Anindya Dutta. Microarray Analysis of DNA Replication Timing. *Methods in Molecular Biology*. 2009;556:191-203. ISBN: 978-1-60327-191-2, Humana Press. PMID: 19488880

Refereed Journal Articles:

- Mignon A. Keaton, Christopher M. Taylor, Ryan M. Layer, and Anindya Dutta. Nuclear Scaffold Attachment Sites within ENCODE Regions Associate with Actively Transcribed Genes. *PLoS ONE*. 2011 Mar 14;6(3):e17912. PMID: 21423757

- Nan Deng, Adriane Puetter, Kun Zhang, Kristen Johnson, Zhiyu Zhao, Christopher Taylor, Erik K. Flemington, and Dongxiao Zhu. Isoform-level microRNA-155 target prediction using RNA-seq. Nucleic Acids Research. 2011 May 1;39(9):e61. PMID: 21317189
- Zhen Lin, Guorong Xu, Nan Deng, Christopher Taylor, Dongxiao Zhu and Erik K Flemington. Quantitative and qualitative RNA-seq-based evaluation of Epstein-Barr virus transcription in type I latency Burkitt's lymphoma cells. *Journal of Virology*. 2010 Dec;84(24):13053-8. PMID: 20943983
- Guorong Xu, Claire Fewell, Christopher Taylor, Nan Deng, Dale Hedges, Xia Wang, Kun Zhang, Michelle Lacey, Haitao Zhang, Qinyan Yin, Jennifer Cameron, Zhen Lin, Dongxiao Zhu & Erik K Flemington. Transcriptome and targetome analysis in MIR155 expressing cells using RNA-seq. *RNA*. 2010 Aug;16(8):1610-22. PMID: 20584899.
- Neerja Karnani, Christopher M. Taylor, Ankit Malhotra and Anindya Dutta. Genomic study of replication initiation in human chromosomes reveals the influence of transcription regulation and chromatin structure on origin selection. *Molecular Biology of the Cell.* 2010 Feb;21(3):393-404. PMID: 19955211.

Refereed Conference Papers:

- Joseph R. Coco, Erik K. Flemington, and Christopher M. Taylor. PARSES: A Pipeline for Analysis of RNA-Seq Exogenous Sequences. *ISCA 3rd International Conference on Bioinformatics and Computational Biology*, New Orleans, LA, March 2011.
- A. Murat Eren, Michael J. Ferris, and Christopher M. Taylor. A Framework for Analysis of Metagenomic Sequencing Data. *Pacific Symposium on Biocomputing.* 2011:131-41. Kohala Coast, Hawaii, January 2011. PMID: 21121041

Presentations

Conference Talks:

- Joseph R. Coco, Erik K. Flemington, and Christopher M. Taylor. PARSES: A Pipeline for Analysis of RNA-Seq Exogenous Sequences. *ISCA 3rd International Conference on Bioinformatics and Computational Biology,* New Orleans, LA, March 2011.
- A. Murat Eren, Michael J. Ferris, and Christopher M. Taylor. A Framework for Analysis of Metagenomic Sequencing Data. *Pacific Symposium on Biocomputing (PSB 2011)*, Fairmont Orchid, Kohala Coast, Hawaii, January 2011.

Posters:

- A. Murat Eren, Marcela Zozaya-Hinchliffe, Christopher M. Taylor, David H. Martin, and Michael J. Ferris. Diversity of Gardnerella vaginalis in Heterosexual Couples. *Microbial Communities as Drivers of Ecosystem Complexity.* Breckenridge, CO, March 2011.
- Seokyoung Kang, Mi Young Noh, Christopher M. Taylor, Yeon Soo Han, and Young S. Hong. Two Human Dengue Resistant Genes Are Functionally Conserved in Aedes aegypti. *American Society of Tropical Medicine and Hygiene*. Atlanta, GA, November 2010.
- A. Murat Eren, Michael Ferris, and Christopher Taylor. A Framework for Analysis of Metagenomic Sequencing Data. *Pediatrics Research Day*. Children's Hospital, New Orleans, LA, June 2010.

Invited Talks:

- Christopher M. Taylor. Analysis of Microbial Communities from 16S rRNA Sequencing. *LBRN Workshop on Computational Biology.* Baton Rouge, LA, March 2011.
- Christopher M. Taylor. Microbial Community Profiling and Metagenomic Sequencing. *LSU-HSC Biostatistics Seminar.* New Orleans, LA, October 2010.
- Christopher M. Taylor. DNA Sequence Analysis: Algorithm Development and Tools. *LBRN Workshop on Computational Biology*. Baton Rouge, LA, March 2010.
- Christopher M. Taylor. High-throughput Sequencing: Algorithms and Applications. *LONI All-Hands Meeting.* Baton Rouge, LA, February 2010.

- Christopher M. Taylor, Neerja Karnani, Ankit Malhotra, and Anindya Dutta. Analyzing DNA Replication Timing in the Human Genome. *Pediatrics Research Day*. New Orleans, LA, June 2009. *Won Best Presentation Award.*

External Funding

Received

- PI: Christopher M. Taylor. Title: Taylor Professional Services Agreement. Source: Research Institute for Children. Amount: $30,349.18. Approved: April 2011. Funding Period: May 22, 2011 to August 14, 2011.
- PI: Christopher M. Taylor. Title: *Pure Sequence-based Classification for Microbial Communities*. Source: UNO Office of Research and Sponsored Programs. Amount: $12813. Approved: March 2011. Funding Period: May 30, 2011 to July 28, 2011.
- PI: Christopher M. Taylor. Title: Undergraduate Student Services Agreement (Manuel Zubieta). Source: Research Institute for Children. Amount: $2250. Approved: Feb 2011. Funding Period: January 31, 2011 to May 21, 2011.
- PI: Christopher M. Taylor. Title: Undergraduate Student Services Agreement (Jonathan Brown). Source: Research Institute for Children. Amount: $2250. Approved: Feb 2011. Funding Period: January 31, 2011 to May 21, 2011.
- PI: Christopher M. Taylor. Title: *Graduate Student Services Agreement* (A. Murat Eren). Source: Research Institute for Children. Amount: $28,061. Approved: May 2010. Funding Period: April 1, 2010 to May 21, 2011.
- PI: Christopher M. Taylor. Title: *Graduate Student Services Agreement* (Joseph Coco). Source: Research Institute for Children. Amount: $21,246. Approved: May 2010. Funding Period: May 17, 2010 to May 21, 2011.
- PI: Christopher M. Taylor. Title: *Graduate Student Services Agreement* (Qi Zhang). Source: Research Institute for Children. Amount: $32,490. Approved: July 2009. Funding Period: August 16, 2009 to May 14, 2011.
- PI: Christopher M. Taylor. Title: *Taylor Professional Service Agreement*. Source: Research Institute for Children. Amount: $7,106.19. Approved: May 2010. Funding Period: May 16, 2010 to August 14, 2010.
- PI: Christopher M. Taylor. Title: *Spring 2010 Professional Service Agreement*. Source: Research Institute for Children. Amount: $13,530. Approved: January 2010. Funding Period: January 4, 2010 to May 15, 2010.
- PI: Erik Flemington, coPI: Dongxiao Zhu, coPI: Christopher Taylor, coPI: Kun Zhang. Title: *Administrative Supplements Providing Summer Research Experiences for Students and Science Educators.* Source: National Institutes of Health. Supplement to *Analysis of Epstein Barr virus type III latency on cellular miRNA gene expression.* Amount: $216,386. Approved: May 2009. Funding Period: June 01, 2009 to August 30, 2010.
- PI: Christopher M. Taylor. Title: *Summer Salary Professional Service Agreement.* Source: Research Institute for Children. Amount: $24,468.89. Approved: March 2009. Funding Period: May 17, 2009 to February 16, 2010.

Dr. Rachel Vincent-Finley, SUBR, Toward the molecular dynamics simulation of multilayer (SiO_2/Ta_2O_5) coatings

Research Interests
Computational and Applied Mathematics

Research Projects
Toward the molecular dynamics simulation of multilayer (SiO_2/Ta_2O_5) coatings

The primary goal of this project is to develop an on-site predictive means for gaining insights into the microscopic mechanisms that lead to mechanical losses in the Laser Interferometer Gravitational Wave Observatory (LIGO) optical coatings having applications beyond Advanced LIGO. [5] [17] In particular, we seek to predict materials properties and performance by building effective computational models of the coatings structures based upon experimentally determined features of the system such as element concentration, valence and charge transfer, bond lengths and number and type of nearest neighbors. The need for, and interest in, modeling of coatings within LIGO has been demonstrated and has applications within advanced versions of gravitational-wave interferometers. [7]

This project complements the existing program of within the Southern University (SU) LIGO Physics Group materials characterization which will continue to make use of neutrons and X-rays as probes and atomic force microscope (AFM) surface imaging at or near the nanometer scale level. The historical emphasis on experimental determinations of chemical composition and microscopic structural studies of multilayered dielectric mirror coatings will be maintained through the use of X-ray absorption spectroscopy methods. [6] X-ray fluorescence (XRF), X-ray Near Edge Structure (XANES) and Extended X-ray Absorption Fine Structure (EXAFS) will be employed to obtain information on chemical composition, valence and charge transfer, bond lengths and number and type of nearest neighbors. This project is intended to expand and undergird the current experimental effort led by Stephen McGuire, Ph.D., Professor, Department of Physics, SU, and in doing so strengthen the ability to contribute to LIGO science beyond Advanced LIGO. [7] In an effort to facilitate this research, Dr. Vincent-Finley requested membership in the LIGO Scientific Collaboration (LSC) and was approved as a senior member by a majority vote of the LSC Council at its March 16, 2011, Council meeting.

The initial focus of the research is to perform *ab initio* molecular dynamics simulations on Ta_2O_5 polymorphs to gain insight into mechanical loss attributes. [14] We study the systems sensitivity to variations of simulation parameters such as temperature, concentration of molecular mixture, and an introduction of external forces. These studies will assist in experimental design and allow us to test extreme conditions (such as temperature of external force load) that may provide further insight into the properties of the coatings.

A database of crystalline ditantalum pentoxide (Ta_2O_5) polymorphs was constructed and preliminary structural studies were performed. Coordinate files for various phases of Ta_2O_5 were constructed using the crystal structure information provided in the literature (for example [1], [2], [4], [8], [12], [13], [16]-[23]). Simulation studies were performed to stabilize these structures.

Some structures that are under consideration include a stable low temperature variant of Ta_2O_5 (L–Ta_2O_5) in the orthorhomic phase reported by Stephenson and Roth. [20] The unit cell contains eleven formula units (22 Ta and 55 O atoms) built with TaO_6 and TaO_7 molecules. In our present work, we are considering a simplified version of this structure. Ramprasad presented a simplified model based on the orthorhombic phase to study oxygen vacancy in Ta_2O_5 and noted that the local environment of Ta is analogous to that of amorphous Ta_2O_5 films. [18] The building blocks of the simplified model are also TaO_6 and TaO_7 molecules, however the unit cell only contains two Ta_2O_5 formula units (4 Ta and 10 O

atoms). A stable crystal structure of high temperature (H–Ta_2O_5) was proposed by Stephenson and Roth based on a study of Ta_2O_5 crystals doped with 2 mole percent of Sc_2O_3. [21]

Other phases of H–Ta_2O_5 under consideration include structures proposed by Liu *et al.*, who present crystal structures of pure H–Ta_2O_5. [13] The crystal structures presented in Liu's work do not rely on doping to assist in the formation of crystalline Ta_2O_5, a distinction that separates the work from its predecessors (see for example [21]).

The current project studies the structural and mechanical properties of Ta_2O_5. The next phase will include Ta_2O_5 and TiO_2 molecular mixtures within multilayer dielectric mirror coatings. These simulation studies are aimed to enhance the study of the chemical and structural behavior of the mirror coatings under laser bombardment. Reductions in mechanical loss have been observed as a function of doping with TiO_2. [7] A LONI allocation is in use to conduct the simulation studies.

The simulation studies are in collaboration with, Hai-Ping Cheng, Ph.D., Professor of Physics at the University of Florida. This work complements the broader work of the LIGO Optics Working Group (OWG) led by Gregory Harry, Ph.D., Research Scientist in the Kavli Institute for Astrophysics & Space Research at MIT.

Abbreviated References.

[1] G. B. Alers, D. J. Werder, Y. Chabal, H. C. Lu, E. P. Gusev, E. Garfunkel, T. Gustafsson, and R. S. Urdahl. "Intermixing at the tantalum oxide/silicon interface in gate dielectric structures". *Applied Physics Letters*, 73(11):1517–1519, September 1998.

[2] Osama A. Azim, M. M. Abdel-Aziz, and I. S. Yahia. "Structure and optical analysis of Ta_2O_5 deposited on infrasil substrate". *Applied Surface Science*, 255:4829–4835, 2009.

[3] R. Car and M. Parrinello. "Unified Approach for Molecular Dynamics and Density-Functional Theory". *Physical Review Letters*, 55(22):2471-2474, November 1985.

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Publication

C. A. Roach, S. L. Neal and R. E. Vincent-Finley, "Matrix Methods in Analytical Spectroscopy", *Encyclopedia of Analytical Chemistry*, eds R.A. Meyers, John Wiley: Chichester. DOI: 10.1002/9780470027318.a9081, (22 pages), December 15, 2010.

Presentation

R. E. Vincent-Finley, "Modeling and Simulation of Multilayer (SiO_2/Ta_2O_5) Coatings"*, All Collaboration Plenary, LSC – VIRGO March 2011 Meeting, March 14 - 17, 2011, Arcadia, California.
* This work was supported by NSF Grant No. PHY-0701652.

Education and Training

Workshop Title: "Computational Science Workshops for Louisiana Educators"
Coordinators: Berta E. Rodriguez-Milla (LSU), Kathryn Traxler (LSU), Rachel Vincent-Finley (SU)
Dates: 07/19/2010 – 07/23/2010
Location: Louisiana State University
Funded by: Louisiana Board of Regents – EPSCoR RII
Website: https://www.cct.lsu.edu/LAeducator

Dr. Collin Wick, LA Tech, Develop and Usage of Computational Methods to Study Interfaces and Carbon Dioxide Sorption

Research Group Members:

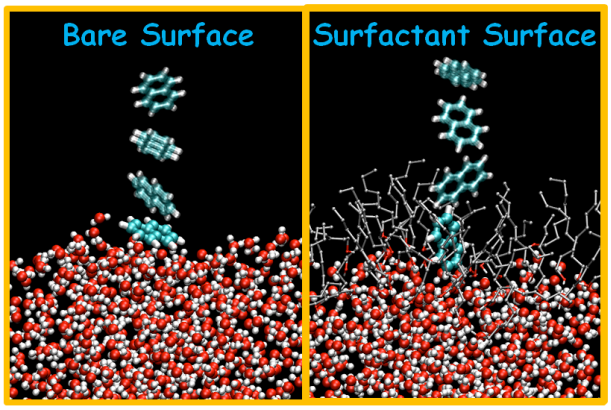
Hui Wu, Oneka Cummings, Shuo Yao, Graduate Students
Josh Slocum, Undergraduate Student

Research Interests

Theoretical Chemistry

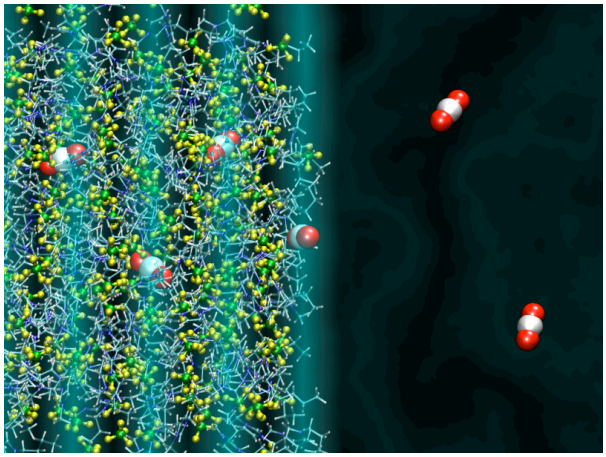
Research Projects

My research focus during the last year has been on understanding the behavior of aqueous interfaces and how different materials absorb carbon dioxide. My work on interfaces has focused on how different species are affected by the type of interface, and what other molecules are present. For instance, of importance to Louisiana is the influence of the remnants of petrochemicals on the ability of fog and mist droplets to scavenge biproducts from many combustion processes called polyaromatic hydrocarbons (PAHs) [1]. This is very relevant to Louisiana due to the large petrochemical present here, previous work finding that fog droplets contain a certain amount of oils [2], and the recent oil split, which could result in a greater amount of oils in the atmosphere. Our work found that the presence of oils on the surface of droplets enhances their ability to scavenge PAHs (see figure), changes their orientation at the surface, which will most likely influence the reactivity of the PAHs, which can make them carcinogenic. This work was the first in a collaborative effort between computational (Bin Chen) and experimental (KT Valsaraj) researchers at LSU and me, and resulted in a publication that was featured on the journal cover [3]. We will be submitting a proposal to further this research, including an experimental component, to the NSF in the summer of 2011. Further work as looked at the behavior of ions at the air-liquid interfaces of water and methanol. Some anions were found to have greater interfacial concentration than in the bulk at the air-water interface, but these same ions did not show similar behavior at the air-methanol interface. This was found to be due to the unique structure of methanol, which allows small hydrophobic pockets to form in the bulk, mimicking some properties found at the air-water interface.



My work examining how different materials absorb carbon dioxide is of significant importance to the Department of Energy, and is a collaborative effort with Pacific Northwest National Laboratory, which provided funds for this work. The goal of this work is to find new strategies for absorbing carbon dioxide from flue gases from coal gasification or other fuel streams. The key is to enhance carbon dioxide absorption to a maximum degree in an efficient manner. Room temperature ionic liquids show promise for carbon dioxide capture, but need to have their carbon dioxide solubility enhanced [4]. Our work looked at it from a different perspective. Instead of investigating the solubility of carbon dioxide in a bulk liquid, we investigated the interface itself, and found that there were pockets of very high solubility in a typical room temperature ionic liquid at the interface.

This work resulted in a publication that was featured on the journal cover [5]. The adjacent figure shows pictorially the pockets of high solubility. If a nanostructured environment could be created, it could significantly enhance carbon dioxide solubility in this ionic liquid. Other work in this area of research has investigated how changing the ionic liquid influences these properties. Additionally, we investigated the ability of metal organic frameworks (MOFs) that were recently synthesized by out collaborators to absorb different hydrocarbon gases on the molecular level. These investigations can lead to a better understanding of how to build MOFs to maximize their absorption of some gases over others, which can be used for energy storage and capture.



All of the described research made great usage of LONI resources, in which around two million computer hours were used. All calculations were carried out on parallel computers, and part of my research is to develop new codes for the simulation of liquids and to make existing codes more efficient. This has spawned a collaboration with Steve Rick at University of New Orleans to create a parallel code to run his code (which runs in serial), so he can exploit LONI resources. Furthermore, the codes I am developing are being used by other researchers in Louisiana to carry out new and more complicated molecular simulations efficiently in a manner that exploits Louisiana's cyberinfrastructure. Currently, I am mentoring three graduate students, who are working towards a PhD (one in engineering and two in computational analysis and modeling), and I have mentored one undergraduate student in research throughout the school year and into the summer. Some of the undergraduate work is to develop modules that can be used to describe simple systems on the molecular level to K-12 students. An example of this is examining how a microwave heats up the surface of water, and how this heat moves through the water. We are developing a way to visualize the water molecules and to simulate microwave action on water. This is part of a new outreach effort being carried out.

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Publications

- C.D. Wick, B. Chen, and K.T. Valsaraj, 'Computational investigation of the influence of surfactants on the air-water interfacial behavior of polycyclic aromatic hydrocarbons,' *J. Phys. Chem. C*, 114, 14520-14527 (2010), Cover article.
- C.D. Wick, T.-M. Chang, and L.X. Dang, 'Molecular mechanism of CO_2 and SO_2 molecules binding to the air/liquid interface of 1-butyl-3-methylimidazolium tetrafluoroborate: A molecular dynamics study with polarizable potential models,' *J. Phys. Chem.B*, 114, 14965-14971 (2010) , Cover article.
- X. Sun, C.D. Wick, and L.X. Dang, 'Computational study of ion distributions at the air/liquid methanol interface,' *J. Phys. Chem.* published online.
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Presentations (all invited)

- C.D. Wick, "The Importance of Polarizability and its Implementation for Understanding Aqueous Interfacial and Bulk Ion Solvation," Invited Talk, CECAM workshop, Lausanne, Switzerland (6/10).
- C.D. Wick, "Ions, ion pairing, and how aqueous interfaces influence them," Telluride workshop on Ions in Aqueous Solutions and Molecular Biology, Telluride, CO, (07/10).
- C.D. Wick, "The Importance of Polarizability and its Implementation for Understanding Aqueous Interfacial and Bulk Ion Solvation," Invited Talk, PacificChem 2010, Honolulu, HI (12/10).

External Funding

- 2010: PI, "Simulations Of CO2 Capture In Ionic Liquids," Battelle Memorial Institute, Richland, WA, $21,075.
- 2010-2015: Senior Researcher, "Louisiana Alliance for Simulation-Guided Materials Applications," National Science Foundation, $20 million to LA, $3.6 million to LA Tech.
- 2010-2012: PI "Computational design of CO_2-philic hydrocarbon polymers to promote more efficient oil recovery," Petroleum Research Fund $50,000.

LI Computational Scientists

Dr. Hideki Fujioka, Tulane

Research Projects

Leveraging Many Jobs To Enable High Performance High Throughput Simulations on LONI and the TERAGRID.

PI: Thomas C. Bishop (CCS, Tulane University)
CS: Hideki Fujioka (CCS, Tulane University)
Rajib Mukherjee (CCS, Tulane University)
Abhinav Thota (CCT, LSU)
Shantenu Jha (CCT, LSU)

Our aim is to investigate sequence dependent variations in the nucleosome using molecular dynamics simulations. Our workflow was inspired by NAMD-G (Gower, et al., 2006). We currently have large TERAGRID (8,000,000SU, June 2010 to July 2011) and LONI (2,000,000SU Jan 2011 to Dec. 2012) allocations that are expected to produce some 50Tb of data.

Our computational challenge is to perform multiple ensemble MD simulations over multiple supercomputers. The simulations consist of M trajectories and each trajectory is divided into N serial tasks that need to be computed one-by-one. In total there are MxN Tasks to be computed using R number of supercomputers.

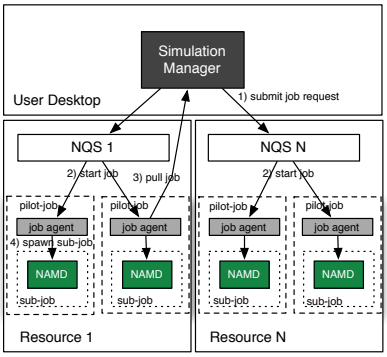


Fig.1: ManyJobs/py Architecture.

The concept of a pilot-job decouples the task/workload execution from resource assignment, in that a pilot-job is submitted without assigning any specific tasks upfront. Actual executable tasks are pulled (or pushed) from a task list after the pilot-job becomes active. LI CS Hideki Fujioka has developed a single task pilot-job, called ManyJobs/py that is written in python (>=2.4) scripts only. SSH (or GSISSH) is used for communication so user has to set up authentication keys. First of all, ManyJobs/py simulation manager (user desktop) submits multiple jobs on multiple resources using SSH. The task descriptions was submitted to a data-base; ManyJob/py is used to launch agents (ManyJob/py job agents) on all resources, which when they became active pulled tasks from the database. When the task is completed, the ManyJobs/py manager submits a new job onto the resource. If a task is set to depend on other incomplete task, the dependent task won't be assigned until the first task is done. If there are no tasks ready to run but still remaining tasks which depend on other incomplete tasks, the job is finalized without pulling any tasks and the submission of new job is suspended. The submission of new job resumes when some running task completed and the following tasks become ready to run.

Figure 2 demonstrates how ManyJobs/py distributed multiple tasks over 6 computing resources. Each colored rectangle represents actual task ran on the resource that the vertical axis indicates. Resources 1~5, which are LONI Linux clusters allow maximum 4 jobs to run concurrently so that there are 4 levels of vertical space within each. For the resource 6, which is TACC Lonestar, we had at most 7 concurrent jobs. The simulation consists of 34 independent task threads and 11 dependent tasks in each thread. However some tasks were not run properly so there are 22 threads presented in Figure 2. The rectangles with same color are dependent tasks in a thread so there are 22 different colors. The number in each

rectangle represents the sequence number of the tasks within a thread. The sequence number begins with 0 and increases up to 10.

In ManyJobs/py each time a job becomes active in some resource, the job-agent pulls a task from the database in the simulation manager. The sequence of tasks in each thread is interleaved across the resources and the following task began running almost immediately after one ahead completed. For example, for the thread with gray-color, where task 0 (the first task in the thread) began running on resource 4 (third from top within resource 4), the dependent tasks 1~6 ran on resource 6, and tasks 7~10 ran on resource 5. These behaviors weren't scheduled prior to the ManyJobs/py initiated. Some thread did not finish the sequence of 11 tasks due to failure of task completion; failures occurred for several reasons, e.g., computation failure, failure of file transfer, communication problems due to network failure etc. We listed 6 resources on the resource database of ManyJobs/py but some resources were not available for some period of time. The resource 6 was unavailable for time=17~68 (hr) for some reason. The resource 2 was unavailable during the simulation period so that no tasks ran at all. The resource 1 was relatively crowded during the simulation. The resources 1~5 only allow 4 jobs to run concurrently due the policy of the site even though ManyJobs/py submitted at most 6 jobs into the queue.

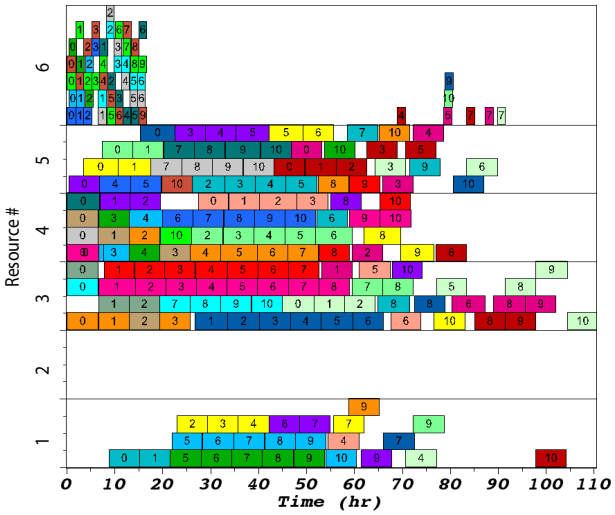


Figure 2: Tasks distributed over 6 supercomputers by ManyJobs/py.

We established the ManyJobs/py developer's *svn* and *trac* site on the CCS Tulane and the web site on http://dna.ccs.tulane.edu/ManyJobs/

External Funding
NIH R01GM076356

Presentation/Talks

- Rajib Mukherjee, Shantenu Jha, Abhinav Thota, Hideki Fujioka, Thomas C. Bishop, "Running Many MD Simulations on Many Super Computers" at 4th LBRN Computational Biology Workshop, March 18th and 19th 2011, Baton Rouge
- T.C. Bishop and R. Mukherjee, "Nucleosomal DNA, kinked, not kinked or self-healing material" at Joint SE/SW Regional ACS Meeting, New Orleans, LA, December 2010
- Rajib Mukherjee, Thomas C Bishop, "Computational Study of Nucleosome Positioning and Stability" at 2011 Annual meeting of Biophysical Society, Baltimore.
- Rajib Mukherjee, Hideki Fujioka, Abhinav Thota, Shantenu Jha, Thomas C. Bishop, "The Nucleosome Simulator: 100 Nucleosomes; 2 Microseconds and Counting", Albany 2011: The 17th Conversation, June 14-18, 2011
- R. Mukherjee and T.C. Bishop. Nucleosomal DNA, kinked, not kinked or self-healing material, to appear in Frontiers in Nucleic Acids an ACS Symposium Series (under review), edited by Richard D. Sheardy 2011

Computational Model of Pulmonary Small Airway Interdependence

Hideki Fujioka, Center for Computational Science, Tulane University
David Halpern, Department of Mathematics, University of Alabama, Tuscaloosa
Donald P. Gaver, Biomedical Engineering Department, Tulane University

Pulmonary airways are surrounded by parenchyma that consists of numerous alveoli, all of which are connected to distal airways. Therefore, the dynamics of each airway and alveolus is interdependent. As such, the behavior of one component may affect all others through parenchymal tethering. The lungs airway tubes are lined with a thin liquid film. Surface tension induces liquid flows, which may cause airways to close due to the formation of a liquid plug if the liquid film is sufficiently thick. Once the plug is created (atelectic), it propagates through the airways as the lung inflates/deflates. Since the flow resistance of atelectic airways is much higher than one with air, the atelectic airway deforms significantly, which may cause high membrane strain in the parenchyma airway tissues. The parenchyma consists of numerous alveoli, all of which are connected to distal airways. Therefore, the dynamics of each airway and alveolus are interdependent. The purpose of this study is to create a model of the lung parenchyma-tethering airway and to investigate the strain of parenchyma during inflation/deflation processes of airways and alveoli.

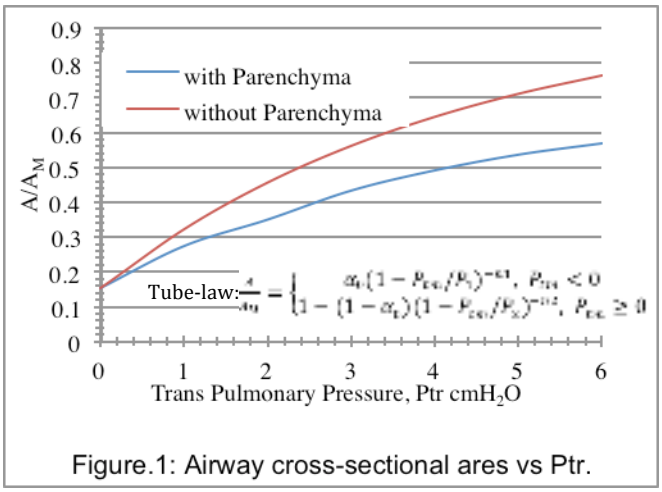


Figure.1: Airway cross-sectional ares vs Ptr.

This project is on the collaboration between Tulane University and University of Alabama. LONI Computational Scientist Hideki Fujioka has developed the model programing and investigated on LONI Linux clusters.

The parenchymal model proposed by Dale et al. (1980) consists of a number of truncated-octahedron alveolar models, which is a 14-sided polyhedron with 8 hexagonal and 6 square faces. Each face consists of septal border fiber bundles that lie on the perimeter of the face and cross-linking fiber bundles that lie across the faces. The fiber bundle comprises many elastin and collagen fibers. The displacement-based finite element method is used to analyze large deformation of the airway/alveolar system as a function of airway lumen, alveolar and pleural pressures as well as tissue constitutive relationships. The tube-law proposed by Lambert et al. (1982) is used to model the luminal cross-sectional area, A as a function of the transmural pressure of airway, P_{tm}.

The trans-pulmonary pressure is defined as $Ptr = P_{ALV} - P_{PL}$, where P_{ALV} is the alveolar pressure and P_{PL} is the plural pressure. Figure 1 shows A/A_M versus Ptr assuming that the pressures in alveoli and airway are same, $P_{ALV} = P_{AW}$, where A_M is A at TLC, P_{AW} is the airway luminal pressure. For the case without parenchyma, since no surrounding tissue, $P_{tm}=Ptr$, and A/A_M changes more sensitive with Ptr. Figure 2 shows the alveolar shapes and the membrane strain at Ptr=6 cmH_2O. Large strain region appears in parenchyma near the airway wall because the airway squeezes the parenchyma outwards that implies $Ptr \neq P_{tm}$. With the tube-law model, we can investigate the local membrane strain at various pressure values in airway, plural and individual alveoli. The mechanism of high alveolar membrane strain

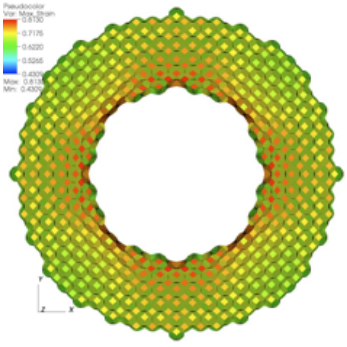


Figure.2: Model shape at Ptr=6cmH_2O

during liquid occlusion of airway and its reopening process will be discussed.

Presentation/talks

- Fujioka, Halpern and Gaver, "Computational Model of Pulmonary Small Airway Interdependence ", Biomedical Engineering Society, 2010 Annual Meeting, October 6-9, Austin Texas.
- Fujioka, Halpern and Gaver, "Alveolar Membrane Strain Distribution near Deformed Lung Airways", Biomedical Engineering Society, 2011 Annual Meeting, October 12-15, Hartford Connecticut.

Distributed GIS Computing for High Performance Simulation and Visualization

PI: Chris Seker (DQSI, LLC, (Dr. Shelly Stubbs))
CS: Hideki Fujioka (CCS, Tulane)
Martin Klein (DQSI, LLC)
Ioannis Georgiou (Director Coastal and Environmental Hydraulics, UNO)

The challenge addressed in this research is to develop new methods for automating the access and processing of raw sensor data, sharing data and methods among researchers, and integrating visualization throughout the process. To meet this challenge, we will develop two new innovations: 1) Geo-Cloud, and 2) COAST HPGIS.

Geo-Cloud is the distributed network environment that maintains connectivity between a Geo-Browser and Geo-Resources (sensor data, GIS datasets, models, simulations, and metadata). The Geo-Cloud maintains all metadata (and ontology) required to efficiently catalog, locate, store, access, and update Geo-Resources. The significance of the Geo-Cloud creation is that it is a highly performing, scalable, network environment that encompasses: 1) a high performance cloud computing (HPCC) environment, and 2) geographical context (HPGIS) whereby users can store, access, and manipulate geographical resources.

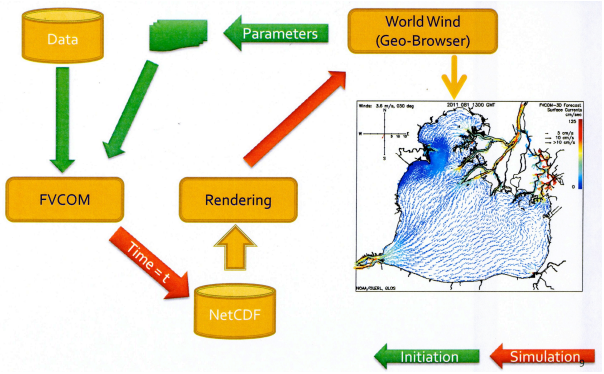


Fig.1: FVCOM Geo-Cloud Integration

COAST HPGIS is an enhanced version of the NASA COAST product which is based on the NASA World Wind geo-browser. COAST HPGIS includes plug-ins, overlays, and interfaces for COAST in order to enable interaction with the Geo-Cloud for real-time visualization of temporal and parametric simulations and models.

For the first phase, we chose FVCOM as a Geo-Resource model and incorporate it into Geo-Cloud system. FVCOM is an open source coastal ocean circulation model developed by UMASSD-WHOI joint efforts. (http://fvcom.smast.umassd.edu/FVCOM/index.html) The model consists of momentum, continuity, temperature, salinity and density equations and is closed physically and mathematically using turbulence closure submodels. The horizontal grid is comprised of unstructured triangular cells and the irregular bottom is presented using generalized terrain-following coordinates. FVCOM was originally developed for the estuarine flooding/drying process in estuaries and the tidal-, buoyancy- and wind-driven circulation in the coastal region featured with complex irregular geometry and steep bottom topography. FVCOM is written with Fortran 90 with MPI parallelization.

We confirmed the FVCOM works on LONI Linux clusters with the Open-MPI library and it scales good. LI Computational Scientist, Hideki Fujioka will tweak the FVCOM source code to integrate into Geo-Cloud.

External Funding
NASA (Under SBIR Program), $100k Phase I Grant; $2.5k LED Phase 0 Grant

Large-Scale Combustion Simulations with Detailed Reaction Chemistry

PI: Ingmar M. Schoegl, (ME LSU)
CS: Hideki Fujioka (CCS Tulane)
Mohsen Ayoobi (ME LSU)

Numerical simulations of reacting flows with detailed chemistry are an important field of research, as they reveal details of chemical processes that cannot be assessed with experimental methods. Combustion simulations with detailed chemistry are computationally challenging, as modern reaction mechanisms involve hundreds of molecular species participating in thousands of chemical reactions. In computational fluid dynamics (CFD), concentrations of individual species add to the parameter space, producing large amounts of data even for relatively small computational grids. Furthermore, combustion occurs in thin reaction layers, which requires suitable grid refinement strategies. The proposed project involves the parallelization of a serial combustion code that is part of Cantera, an opensource chemistry package. (http://code.google.com/p/cantera/) The scope of the project is to investigate laminar, premixed combustion on one/two/three dimensional domain using large reaction mechanisms.

The LONI Institute Computational Scientist, Hideki Fujioka helps a PhD student at LSU, Mohsen Ayoobi to identify the best approaches for building a parallel framework for large-scale combustion simulations that is suited for 1D, 2D and 3D domains. We have confirmed the chemistry package, Cantera works on LONI Linux clusters. For grid/mesh, Deal.II, adaptive mesh refinement and finite-element differential equation analysis library will be used. (http://www.dealii.org) We will use Deal.II to develop a model equation solver incorporating with the Cantera. C++ is the main programing language and python is used for preprocess and post-process.

We will develop sequential codes for solving 1D diffusion equation w/wo convection and/or reaction terms. The Deal.II provides the method to discretize differential operators and the method to create appropriate linear systems. These methods are designed for problems of more than one dimension. In next step, the code for the convective-diffusion equation for temperature and single species (i.e. conservation of energy and mass) will be developed. In this case, the density is one of unknown variables and should be solved with an ideal has equation. Non-linear PDE solver on Deal.II/Petsc is required. We will create a C++ class to handle read/write access for temperature and species concentrations in each grid point. This class can be adapted to different underlying data structures. (i.e. generic parent class with functions that can be overloaded to handle data from deal.II, PetSc, etc.) The Convection-diffusion equation for multiple conserved quantities (temperature; and arbitrary number of species) will be solved. The code should work through a Cantera interfaces to pass variable coefficients (density, diffusivity, viscosity etc.). Once sequential codes work, we will modify the codes to compute in parallel. Deal.II provides Petsc interfaces, which we can use without changing whole code structure. We use svn for version control and doxygen-style comments in the codes. Result output format will be in VTK format (may need MATLAB routines to read 1-D data).

External Funding
Louisiana BoRSF RCS grant LEQSF(2010-2013)-RD-A-04

Dr. Raju Gottumukkala, ULL

Research Group Members:

Dr. Ramesh Kolluru, Director, NIMSAT Institute and CBIT
Dr. Mark Smith, Professor and Head of Department of Moody College of Business Administration
Dr. John Zachary, Director of Information Systems Research, NIMSAT Institute and CBIT
Dr. Baker Kearfott, Professor, Mathematics Department
Mr. Haochun Zhang, Student

Research Interests

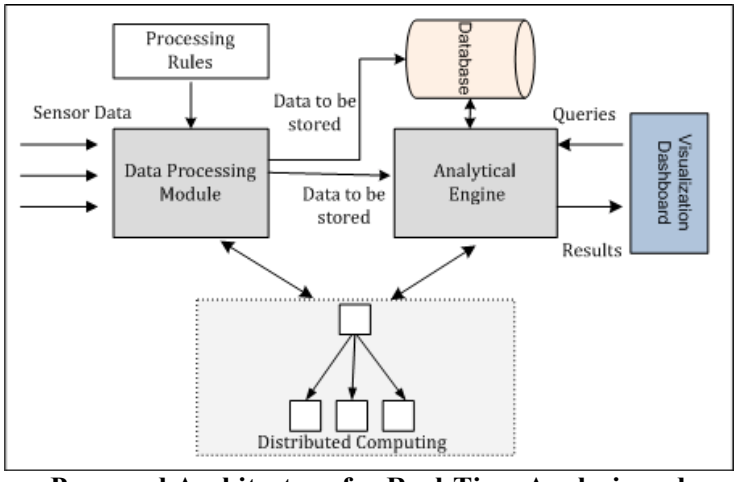
Dr. Raju Gottumukkala is a LONI Computational Scientist at the National Incident Management Systems and Advanced Technologies (NIMSAT) Institute at the University of Louisiana at Lafayette. Raju's research interests include reliability and availability modeling, resource management of large scale parallel applications, parallel algorithms for linear optimization and design of grid based tools and techniques for disaster management. Raju's areas of expertise include distributed systems, service oriented computing, parallel algorithms, probabilistic modeling, and spatiotemporal optimization problems.

Research Projects

A High Performance Data Analytics framework for Large Scale Data Analysis

Dr. Ramesh Kolluru, Dr. John Zachary, NIMSAT nstitute, UL Lafayette
Dr. Vijay Raghavan, Dr. Ryan Benton, Center for Advanced Computer Studies, UL Lafayette

The main goal of this project is development of a distributed data management component and a data analytics component on the federated LONI cyberinfrastructure for large-scale data analysis. Dr. Gottumukkala developed a project proposal titled *"Real-Time Analysis and Visualization of Multi-dimensional Sensor Data"* as the lead PI for the proposed NSF I/UCRC Center for Visual Analytics at University of Louisiana at Lafayette.



Proposed Architecture for Real-Time Analysis and Visualization of Sensor Data

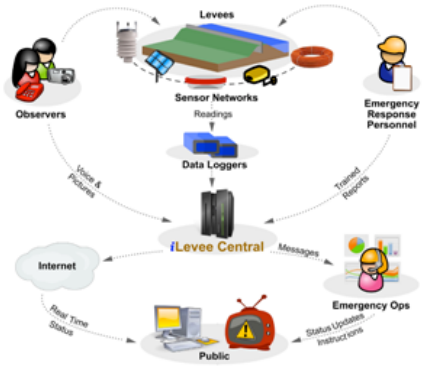
The proliferation of inexpensive sensor devices affords the opportunity to collect and acquire situational awareness, which allows stakeholders to make informed decisions that have significant application in industrial/occupational safety, homeland security, telemedicine, and environment safety among others. These environments are typified by massive amounts of real time, complex data streams, which challenge current methods of data storage, communication, and computation. In this project, we specifically deal with the storage and computational issues. The proposed real time sensor analysis and visualization framework will provide a capability for decision makers to quickly detect and interpret actionable information, such as potential or possible event occurrences, from huge and dynamic data acquired from distributed sensor data sources. This project includes the development of an integrated framework that supports (1) real-time data collection and processing; (2) rapid analysis and visualization of multi-dimensional sensor data; (3) techniques for automated preprocessing and prediction of event

trends by leveraging parallel and distributed computing frameworks; and (4) decision support tools for visualizing data. The figure (to the right of the page) shows the architecture of the proposed framework. As part of this project, Dr. Gottumukkala also assisted with another project titled "Analyzing Social Media Content for Decision Making Based on Event Emergence" as a co-Investigator.

iLevee: Intelligent Flood Protection Monitoring, Warning and Response System

The State of Louisiana Department of Natural Resources, Office of Coastal Protection and Restoration (OCRP) plans to deploy a state of the art Intelligent Flood Protection Monitoring, Warning and Response System (IFPRMWRS) at strategic locations within Mississippi River flood control systems. iLevee is a collaborative project that includes Geocomp Corporation, PB Americas, Shannon & Wilson, James Lee Witt Associates, NIMSAT Institute at the University of Louisiana at Lafayette, SMARTEC and TIE Technologies.

iLevee collects data from monitoring sensors installed throughout the flood control system, Web or Mobile phone based responses from observers in the form of images, voice and text data and processes them in real time to display the health and status of the flood control system. This data is processed in real-time by decision support tools that are hosted on iLeveeCentral to assess the health of the levee and reports the status of levee health to first responders. The iLeveeCentral is the backbone of the iLevee system that consists of various hardware and software to receive and store incoming data streams through the internet, a probabilistic decision support system that runs on LONI and a GIS system that runs on a server to track and display the location of each source of data. In order to make the system highly available and avoid single points of failure, certain components of the system will be deployed at UCSD.



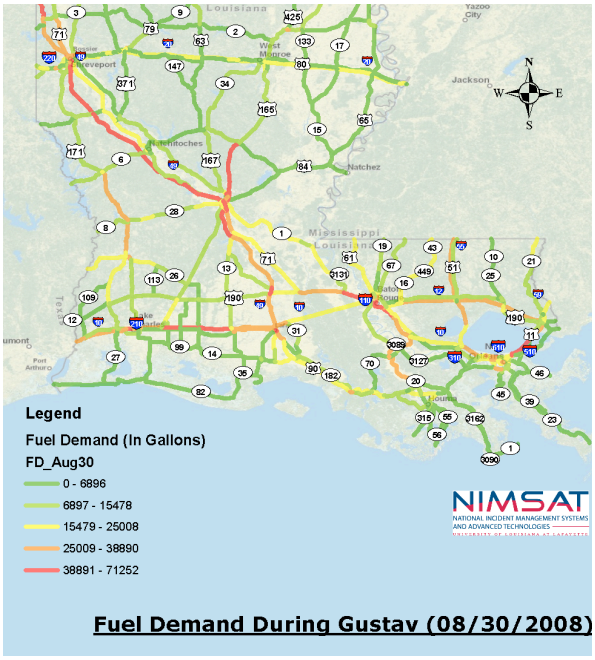
Concept of the iLevee System (obtained from the Proposal)

Dr. Gottumukkala leads the development of the cyberinfrastructure component of the iLevee Central system including the development of the software, data processing and computational modules.

Fuel Demand Estimation for Regional Hurricane Evacuation

One of the primary reasons for severe congestion during large-scale evacuations is the rapid depletion of fuel in the gas stations as people try to fill-up their fuel tanks to get out of harm's way. Unexpected fuel outages have caused hundreds of motorists to be stranded, despite a coordinated effort by state agencies and oil and natural gas partners. In order to prepare and respond to issues related to fuel outages, emergency managers need estimations on the available fuel supply, and fuel demand along various evacuation routes, both prior to and during an event. This would enable the emergency managers to identify critical section of highways and inform the gas station owners on the anticipated fuel demand, send refueling trucks ahead of contraflow, and supply generators the gas stations that are in the critical evacuation paths in the event of a power outage.

Fuel demand to a large extent relies on the evacuation traffic. Evacuation traffic may be estimated from an evacuation planning models or tools that estimates evacuation traffic. The problem of evacuation is typically formulated as a transportation network problem that allocates traffic to evacuation highways based on how people load onto the evacuation highway network, where the destinations are and the shortest travel times to destinations. While there is a body of research in evacuation models and evacuation planning tools, estimating evacuation traffic remains a challenging problem owing to the uncertainty in the hurricane track, the behavior of peoples and the series of events that unfold during an event. Recent research sponsored by the National Science Foundation has revealed that most published evacuation transportation models rely on assumptions that are not consistent with findings of behavioral research on hurricane evacuations. Conversely, behavioral scientists have failed to collect data on various parameters that are important to evacuation traffic modelers.



Map showing the Fuel Demand Estimation along the evacuation routes for Hurricane Gustav

Dr. Gottumukkala along with an interdisciplinary team of researchers from social and behavioral sciences, transportation modelers, mathematics and emergency management practitioners developed a fuel demand estimation model for regional hurricane evacuation for the state of Louisiana's Department of Natural Resources.

All hazard risk assessment for Community Education and Outreach

Dr. Gottumukkala also developed an all-hazard risk index and social vulnerability index based on the spatiotemporal characteristics of historical hazards and socio economic characteristics of various parishes in the state of Louisiana. The all-hazard risk indices and vulnerability indices were developed as a funded project "Community Education and Outreach" for the state of Louisiana's Governor's Office of Homeland Security and Emergency Preparedness.

Recent Publications

- Zhang, Haochun, Kearfott, R. B., Gottumukkala, N.R., and Kolluru, R., "A Multi-Objective Mixed Optimization Model for Points of Distribution to Distributed Emergency Suppliers," submitted to Transportation Research Part E: Logistics and Transportation Review, at the beginning of the peer review process
- Gottumukkala, N.R.; Nassar, R.; Paun, M.; Leangsuksun, C.B.; Scott, S.L., "Reliability of a System of k Nodes for High Performance Computing Applications," Reliability, IEEE Transactions on , vol.59, no.1, pp.162-169, March 2010, doi: 10.1109/TR.2009.2034291
- S. Katz, G. Allen, R. Cortez, C. Cruz-Neira, R. Gottumukkala, Z. D. Greenwood, L. Guice, S. Jha, R. Kolluru, T. Kosar, L. Leger, H. Liu, C. McMahon, J. Nabrzyski, B. Rodriguez-Milla, E. Seidel, G. Speyrer, M. Stubblefield, B. Voss, and S. Whittenburg, "Louisiana: A Model for Advancing Regional e-Research through Cyberinfrastructure," Philosophical Transactions of the Royal Society A, v. 367, pp. 2459-2469, 2009.

Conference Presentations

- N. Raju Gottumukkala, et al. "Real-Time Analysis and Visualization of Multi-dimensional Sensor Data", NSF I/UCRC planning workshop for the Center of Visual and Decision Informatics, Drexel University, Philadelphia, PA.
- N. Raju Gottumukkala, Ramesh Kolluru, Xiaoduan Sun, Mark Smith, Bob Grambling, Haochun Zhang, "Fuel Demand Estimation for Regional Hurricane Evacuation", The National Evacuation Conference, Feb 3-5, 2010, New Orleans, LA.
- N. Raju Gottumukkala, "Improving Disaster Response: NIMSAT", The 2009 Gulf Coast Marine Conference, Sponsored by the National Oceanic and Atmospheric Administration, the National Weather Service, and National Ocean Service,, LITE Center, Lafayette, LA.
- N. Raju Gottumukkala, Risk Assessment Methodology for Louisiana's Hazard Information Portal: Community Education And Outreach, State Hazard Mitigation Planning Committee Meeting, Baton Rouge, LA.

External Funding (As Co-PI or Key Personnel)

- "Dam and Levee Performance and Risk Management Cyber System", Jackson State University / NSF, IMEE, $ 307,377 (2011-2014) (Pending)
- Real-Time Fuel Supply-Demand Modeling for Enhanced Mass Evacuations: A
- Generalizable Goal Optimization Framework, NSF, Infrastructure Management and Extreme Events (IMEE), $ 550,012 (2011 – 2013) (Pending)
- "UICDS Implementation in Louisiana and in the Gulf of Mexico Region", U.S. Department of Homeland Security, $ 499,918 (2010 – 2012)
- "iLevee: intelligent Levee Monitoring System", funded by GeoComp Corporation/Louisiana Office of Coastal Protection and Restoration; $2,981,813 (2010 – 2011)
- "GOHSEP-NIMSAT Institute Cooperative Endeavor Agreement", funded by the Governor's Office of Homeland Security an Emergency Preparedness, $574,992 (2009-2010).
- "Enhancing the State of Louisiana Emergency Operations Plan: Critical Infrastructure & Supply System Interdependency Analysis for Energy Assurance", funded by the US Department of Energy/Department of Natural Resources; $513,998 (2009-2012).
- "Community Education and Outreach (CEO): Public Communication and Hazard Data Management Platform Portal", funded by GOHSEP/FEMA; $825,000 (2008-2011).
- "Parallel-GIS: An Open Source GIS Application on the Supercomputers of LITE and LONI", funded by Governor's Information Technology Initiative; $284,240 (2007 –2010).
- "UL Lafayette Emergency Management for Higher Education", U.S. Department of Education $440,286 (2009 – 2011)

Recent Outreach Activities

- Developed LONI relevant projects for the proposed NSF I/UCRC Center for Visual and Decision Informatics, a collaboration between University of Louisiana at Lafayette and Drexel University.
- Mentoring Haochun Zhang, PhD Student, Department of Applied Mathematics, University of Louisiana at Lafayette
- Organized a LONI Workshop at University of Louisiana at Lafayette
- Assisted with evaluation the HPC systems at the Louisiana Immersive Technologies Enterprise

Dr. Abdul Khaliq, LA Tech

Research Interests

- Semiconductor process and device simulations
- Modeling and simulations of MEMS device fabrication and characterization
- Micro and nano-fluidic devices
- Microelectronics
- Numerical code development and implementation for Finite Difference Method
- Optical and electromagnetic simulation
- Commercial FEM tools, e.g. ANSYS, COMSOL, etc.
- Quantum Computing with Gaussian , Material Studio, etc.
- Scientific computing with MATLAB, Mathematica, etc.
- Metrology instruments, e.g. FESEM
- Semiconductor physics
- Computation of Bio-systems

Research Projects

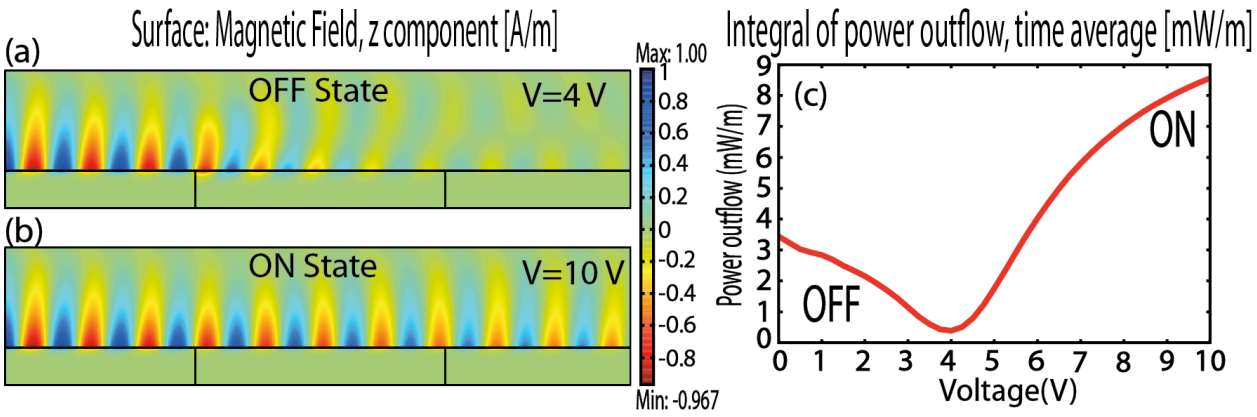
Surface plasmons in metal/semiconductor devices

Dentcho A. Genov, PhD. (LI faculty, Louisiana Tech University)
Abdul Khaliq, MS. (LI CS, Louisiana Tech University)

Background: The proposed research aims to develop novel optical transistors based on surface Plasmon. The preliminary data suggest that this optoelectronic device can provide modulation bandwidth larger than 1THz, which can potentially open a new rout toward fast optoelectronics and computing.

Research Objectives: We intend to develop a novel semiconductor based Surface Plasmon Transistor (SPT). The SPT promises to combine electronics with optics by excitation and active control of propagating surface plasmon modes through Si/GaAs *n-p-n* junction. To study the device characteristics we will seek to integrate commercial software COMSOL, to perform a distributed memory, parallel parametric FDFD electromagnetic simulations on the LONI clusters.

Research Accomplished: The electron generation in a three-layered Si/GaAs device is analyzed with the state of the art semiconductor device simulator "MEDIC". In the device a p-type Si/GaAs is sandwiched between two layers of n-type. We have established an analytical fit for the doping profile in the p-region. A 2D model in COMSOL has been simulated which is shows in the following figure:



Future Work: The future work includes an expansion of this 2D model into full 3D model.
Impact of the Proposed Research: Project is focused on the development of new type of surface plasmon transistor that is far superior compared to the conventional devices in terms of it potential bandwidth scalability. The work initiated in this proposal, is expected to serve as a basis to build on existing and establish new collaborations with theoreticians and experimental scientists within the six LONI institutions.

This is a continuation of the previous year project.

Thermodynamics and Kinetics in H_2 Storage Systems

Weizhong Dai, PhD. (faculty, Louisiana Tech University)
Abdul Khaliq, PhD. (LI CS, Louisiana Tech University)

Background: Among the barriers that hinder the use of hydrogen as a clean alternative to hydrocarbon fuels are absorption/desorption rates, volume/weight ratios, hydride stability, and desorption temperatures of current H_2 storage materials. We will use novel multiscale MD and MC simulations, kinetic MC, finite element, and finite difference modeling to predict rates of hydrogen uptake/release over time scales reaching 10^3 s and extending over use X-ray tomography to probe these materials over the same length and distance scales. The goals of this focus area are to predict the influence of catalytic additives in enhancing mobilities and desorption rates in metal hydrides and to explore a wider range of potential hydrogen storage materials. The payoff will be an improved ability to design materials of hydrogen storage.

Proposed Research: We will study diffusion and reactions using kinetic MC and employ finite element and finite difference methods for extending length and time scales.
- Employ the LSU X-ray synchrotron tomography beamline and the Argonne Advanced Photon Source nanotomography beamline to study in situ and ex situ de/rehydrogenation reactions, to assess 3D microstructures and interphase boundaries, and to quantify the distribution and size of single-phase domains.
- CTCI visualization toolkits will be utilized since atomic diffusion rates may limit the desorption, Browne (LSU) will use Fick's Law diffusion and nonequilibrium chemical models to model solid state diffusion and phase transitions.
- The temperature-dependent diffusion coefficients will be determined using diffusion and diffusion-reactions equations and experiments.

Impact of the Proposed Research:
The results of these simulations, calculations, and experiments will be the prediction of optimum conditions and materials for hydrogen release and uptake.

This is a funded project of Louisiana Alliance for Simulation-Guided Materials Applications
(LA- SiGMA).

Experimental and computational approaches in the development of drug-eluting stent coatings

Tammy R. Dugas (Faculty, Department of Pharmacology, Toxicology, and Neuroscience, Louisiana State University Health)
Abdul Khaliq (LI CS, Louisiana Tech University)

Background: Stents are metal-latticed tubes commonly used to restore blood flow through narrowed arteries due to plaque accumulation associated with cardiovascular disease. Although bare metal stents

(BMS) are still a mainstay in the clinical regimen, drug-eluting stents (DES) are becoming increasingly popular. However, DES pose a unique design challenge, primarily due to the large concentration gradients that are established as drugs are released from the polymeric coating. This flux depends on many variables that are inherent to the drug, polymer, and artery.

Research Objectives: The present study coupled experimentally-defined transport coefficients with computational modeling to gain insight into the pharmacokinetics of two vascular-protective polyphenols, resveratrol (RESV) and quercetin (QUER), after release from a stent platform. Arterial diffusion coefficients specific to RESV and QUER were determined using bovine carotid arteries exposed to radiolabeled RESV and QUER in a Franz diffusion chamber. Arterial distribution was compared to paclitaxel, a drug currently used in clinical DES. RESV and QUER were loaded into polymer coatings to examine *in vitro* release kinetics. Using high performance liquid chromatography we found that elution of RESV and QUER followed biphasic release kinetics, showing an initial burst phase followed by a low-level sustained drug release. Surface diffusion coefficients (D_s) and volume diffusion coefficients (D_v) were defined to describe the initial burst phase and sustained release phase, respectively. This dual-layer polymer assumption was incorporated into a 2-dimensional computational model using experimentally-derived coefficients of drug transport. Our results indicate that the dual-layer approach obtains good agreement between model predictions and experimental observations of RESV and QUER release from polymer films.

Impact of the Proposed Research:
Future studies coupling this methodology to arterial geometry may be valuable in predicting therapeutic tissue concentrations and drug residence time, reducing prototype coating formulations.

LONI-Assisted modeling of brain tumor cell growth in 2- and 3-dimensions

(PI: M. DeCoster)

The proposed project will greatly facilitate modeling of brain tumor cell and normal brain cell growth in 2- and 3-dimensions (2D, 3D) using dynamic cell culture systems for experimental input and assisted by digital imaging and analysis software. Experimental input will come from Louisiana Tech University (LaTech) which has LONI (LI) nodes, and in partnership, we propose to work with LI Computational Scientists (LICSs) to develop computational methods for better visualization and modeling of both normal and diseased brain cell growth. We suggest Dr. Abdul Khaliq as our LICS partner as we have recently published a manuscript together and thus have an excellent and productive history of collaboration **(1).** The genesis for this proposal comes from recently discovered techniques in our laboratory which allow for sustained 3D growth of both normal and tumor brain cells in contiguous cell groups or sphere-like structures (objects). Thus, in our model, each sphere-like structure is maintained as a single object which may be measured in 2 dimensions on a daily basis by non-destructive digital microscopy and image analysis. To date, cultures have been maintained and grown in this system for at least 14 days. In 11 samples analyzed thus far, we have measured on average more than a 300% greater difference in growth area rate for tumor cells vs. normal brain glial cells over a 7 day period. Furthermore, we have measured a large difference in object shape for normal vs. brain tumor cells using our new model. Our computational needs are twofold: 1) computational methods are needed to predict the dynamics of brain tumor object area and shape changes so that potential anti-cancer drug efficacy may be better evaluated; 2) while object growth can be monitored and captured digitally in a non-destructive manner in 2 dimensions in our model, the brain tumor object growth in our model (as well as in reality) is occurring in 3 dimensions, thus computational methods are needed to calculate, infer, or predict volume dynamics from area changes measured and obtained experimentally over time.

We envision a team of researchers at LaTech assisted by LICSs that will work together to iterate experimentally obtained digital images showing a progression of different brain cell growth over time

with computational models for prediction and visualization. LICSs will be an integral part of the research team, and we anticipate that if accepted, this partnership will result in the professional development of LICSs to include co-authorship on meeting abstracts, peer-reviewed publications, and funding in future grant proposals to local and national funding agencies. We therefore request the effort of 4 FTE months for partnership with one or more LICSs on this project, suggesting Dr. Khaliq as a possible candidate for this position. As indicated on cover page, the PI has adequate current funding to support ongoing studies for this project which will ensure productive collaboration with the LICS. In addition to our initial publication together, we are including Dr. Khaliq on a grant proposal (requesting 3 years of funding) to be submitted in mid February 2011 to NSF on this topic of computational methods for brain tumor growth. A second proposal will be submitted in May to NIH for clinical applications using this model and Dr. Khaliq will play a key role there as well. We anticipate that linkage to LONI resources will aid in the overall strength of the proposals to both of these agencies, increasing our changes for external funding.

(1). Khaliq, A., Jenkins, F., DeCoster, M., Dai, W. "A new 3D mass diffusion-reaction model in the neuromuscular junction". *Journal of Computational Neuroscience* pages 1-17 (**2011**) In Press.

Thermal Energy Storage

The proposed work focuses on the prototype design and fabrication of one component of the larger MEMS-based thermal energy harvesting system. The complete system consists of a boiler, thermal energy storage device, and micro-engine as shown in Figure 1.

Basic engine dimensions are on the order of a few millimeters. Output from a single microengine is designed to be on the order of 100 mW. Larger output is possible through multiple engines acting in parallel. The PI, Dr. Weiss, has already commenced boiler development at Louisiana Tech. Novel materials and design are being utilized to enhance boiler performance. These include copper plating for the boiler surface with integrated capillary action channels that continually supply working fluid to the heated surface. The research proposed in this work focuses particularly on the design and prototype fabrication of the thermal energy storage device.

FEM based software COMSL will be used to predict the energy storage while wax melts. Essentially, it is two phase flow problem. In the second stage a metallic grid will be inserted in the model to increase energy storage. Finally, a full three model will be developed for real time simulation of the device.

Publication

- Khaliq, A., Jenkins, F., DeCoster, M., Dai, W. "A new 3D mass diffusion-reaction model in the neuromuscular junction". *Journal of Computational Neuroscience* pages 1-17 (**2011**) In Press.

Book Publication

A book based on my Ph.D. dissertation has been published by LAMBERT academic publishing:

Modeling of Diffusion-reaction System in the Neuromuscular Junction: A Stable and Accurate Finite Difference Method

Brief Description

A new stable and accurate numerical method is used to solve the equations with Neumann boundaries in cylindrical coordinates. The simulation analysis agrees with experimental measurements of end-plate current and agrees well with the results of the conformational state of the acetylcholine receptor as a function of time and acetylcholine concentration of earlier investigations with a smaller error compared to experiments. An asymmetric emission of acetylcholine in the synaptic cleft and the subsequent effects on open receptor population is simulated. Sensitivity of the open receptor dynamics to the changes in the

diffusion parameters and neuromuscular junction volume is investigated. The effects of anisotropic diffusion and non-symmetric emission of transmitter at the pre-synaptic membrane is simulated.

Inter-Institutional Collaboration
Drug elusion project is a collaboration with LSU at Shreveport. It is important project with wide range of applications.
Currently, I am collaboration with Dr. Zhang Le from Michigan Tech University for modeling and simulation of cancer tumor. We also invited Dr. Zhang for a talk at our location.

Student Support and Education
Few of the activities in this regard are listed in the following:

- Trained students for MEMS CAD/TCAD software
- Assisted faculty/students to identify appropriate software for their research
- Helped students to run simulations for research and study
- Proposed efficient virtual experiments to assist lab users to optimize their device design

These are critical areas for the College of Engineering and Science. The training provided for students on software packages that is widely used in the semiconductor industry makes them more employable. I have also developed a short course for process and device simulation using TCAD.

My TCAD expertise also becomes important when college offer courses like ELEN 537/MSE 538. Because of my familiarity with the lab and the software takes a substantial burden off the instructors. I also, delivered a guest lecture for Dr. Wang's class MSE-501 for MEMS process simulation with CAD.

Material Studio Installation on LONI Resources
This year I worked with the LONI sys-admins and managed to get our Material Studio license installed on Painter, the LONI Linux cluster on our campus. This has increased the accessibility of the software and the number of cores on which it can be run, both extremely beneficial for our students. This allows us to run large computationally extensive simulation on Linux clusters. This practice may reduce overloading of our existing workstations intended to be used for short runs. I worked with Dr. Hegab to get FLUENT installed on Painter. I was able to figure out a method to run FLUENT on Painter in parallel.

Research Support
A significant time is spent supporting research activities in the areas which are listed following:

- MEMS
- Microfluidic Devices
- Semiconductor Devices/Microelectronics
- Bio Computing

This is a highly diverse list of disciplines in which I am able to provide guidance and assistance to the students.

Summary
I have focused my efforts in maintaining the computational simulation and modeling labs in Nethken Hall, rendering assistance to students and faculty with software use, participating in teaching by guest lecturing on the use of specific software packages in upper division and graduate courses upon request, and participation in research projects assigned to you by the LI Scientific Team.

Dr. Bhupender Thakur, LSU

Research Interests
Computational materials research using Quantum Monte Carlo among other many-body techniques, bio-molecular research using force field based methods and software development for newer hybrid computational platforms. Parallel code and algorithm development using MPI, OPENMP and CUDA. General scientific programming toolkits.

Roles/Specializations
Forge partnerships and collaborations with LONI and LA-SiGMA faculty.
Improve research merit by scaling problems to national leadership class machines. Provide research and IT support for LONI meetings, seminars and proposals.

Research Projects

Next Generation GPU-Based Codes for Materials Discovery

Collaborators: T. Bishop (Tulane) and D. Mobley (UNO), M. Jarrell, J. Ramanujam, J. Moreno, B. Chen, and R. Hall (LSU) S. Dua (LA Tech), B. Thakur (LONI Institute)
Graduate Students: Kaushik Raghavan, LSU

Role: Co-PI, Initiate new research, develop scalable algorithms and code for large scale parallel and hybrid platforms using MPI and CUDA, and mentor graduate students.

Description:
Due to energy usage, the present generation of parallel computing cannot simply be scaled to the exascale. Nearly all proposals for beyond petascale computing involve heterogeneous computers. In most cases, this involves the use of the General Purpose Graphics Processing Units (GPGPU or GPU) generally running CUDA or OpenCL. Current national leadership class machines at the National Center for Computational Sciences include GPU clusters, and BlueWaters at NCSA will also likely be at least partially heterogeneous. Indeed, GPU acceleration is ideally suited for the Monte Carlo (MC) and Molecular Dynamics (MD) codes used by many investigators. Thus, in order to remain internationally competitive, it is essential for us to both develop GPU accelerated codes and to learn how to use the local and later the national GPU hardware to enable new discovery.

Rationale:
The PIs are particularly well qualified to accomplish the goals of this request. CCT recently purchased a GPU Fermi cluster and about 10 GPU(GT460) based workstations with recently funded LI LA-SiGMA project (insitute.loni.org/lasigma) and will purchase a larger GPU cluster. Efficient migration to and utilization of existing codes on next generation heterogeneous computers is a central component of LA-SiGMA. Drs. Jarrell and Hall have supervised the effort, with help from Dr. Thakur, of 6 undergraduates students over the past 5 months devoted to investigating the issues related to migrating MC codes to GPU machines. Dr. Bishop has strong ties with the creators of NAMD and is in position to evaluate different modes of operation of NAMD on GPUs. Dr. Mobley is involved with a molecular dynamics free energy code, “Yank”, for binding free energy calculations on GPUs, and interacts closely with the developers of the OpenMM library which includes GPU support. LA-SiGMA is composed of 3 “Science Drivers” (correlated materials, energy materials, and bio-molecular materials) which are closely coupled with a computational effort which includes migration to GPUs. Involvement of LI-CS Bhupender Thakur in this effort will have an immediate and beneficial affect on the a large number of researchers within the LI. All of the investigators in this project are also LA-SiGMA investigators. LA-SiGMA had hired MS graduate student Kaushik Raghavan to directly work under the supervision his supervision.

Effort and Progress:
LI-CS currently has six months in the current year assigned to this project as a part of LONI allocations. He is also responsible for the activities of larger group GPU of about 20 personnel, involving several LI faculty (M. Jarrell, J. Moreno, J. Ramanujam to name a few), graduate students (K. Raghavan, S. Abu-Asal, Y. Feng, C. Moore among others) and REU students (J. Caprino, C. Thomasson and S. Williams). He is responsible for organizing and assigning tasks to each individual in the group.

Quantum Monte Carlo for strongly correlated systems

Collaborators: Dr. M. Jarrell and Dr. Juana Moreno (PI, Department of Physics, LSU)

Graduate Students: Shuxing Yang, LSU

Description:
The project implements a new formalism (Dual Fermion) coupled with the existing Dynamic Cluster Approximation (DCA) for investigating strongly correlated systems. The method converges much more rapidly and has been shown to scan efficiently to more than 2000 processors.

Effort and Progress:
Effort is underway to increase the scalability of the method to tens of thousands of processors on supercomputing facilities at ORNL and NERSC. The LI CS is involved in writing allocation proposals and for efficient implementation of parallelization procedures.

Development of force fields for bio-molecular systems

Collaborators: PI: Dorel Moldovan, Mech Eng. (LSU), Co-PI : Hank Ashbaugh, Chem. and Biomol. Eng., Tulane University, Co-PI: Bhupender Thakur(LONI)
Graduate Students: Kumuditha Ratnayake, LSU

Project Description:
The empirical force field used in MD simulations describes the interaction potential energy of a system of atoms or molecules with certain functional terms representing bonded and non-bonded interactions between atoms and a set of parameters characterizing these interactions. Despite of extensive use, and recent developments, not all molecules of interest can be parameterized directly by direct reference to the available, well-established, force field packages, such as AMBER, CHARMM, OPLS, GROMOS, etc. Therefore there is great deal of interest in expanding and streamlining the procedures and methodologies for the development of force-fields and this is the goal of the proposed project. Given the current interest of the PIs in the mechanisms of self-assembly of various amphiphiles into structures that may serve as drug delivery vehicles, the development of a coherent strategy for parameterization of the interactions in such systems is of great relevance.

Goals:
The goal of this project is to develop, and document, an optimized methodology for obtaining accurate force field parameters for a large class of bio-molecules such as: Span80, Phospholipids, bile salts (cholate, glycocholate, taurocholate), etc. The results obtained together with the codes and algorithms developed in this context will be archived and disseminated through publication for greater use by researchers working in this area. Various simulations are currently being performed using GROMACS 4.0 and Amber 10 on LONI computer clusters. Bhupender will work together and provide technical expertise and guidance to Kumuditha Ratnayake a second year graduate student assigned to this project.

Benefits to LONI Institute and scope within LA-SiGMA:
The development of the formalisms and algorithms for force field development will benefit multiple projects at LSU and Tulane, including the collaborative NSF funded project LA-SiGMA. We aim to

further archive the results and provide the algorithms, to all LONI users upon validation. An online resource comprising a compute facility and a database is also being considered for a greater benefit to a larger community

Effort and Progress:
LI-CS currently has five months in the current year assigned to this project as apart of LONI allocations. Preliminary work has been completed by optimizing the AMBER ff03 force field for Span80. Gaussian calculations were carried out to reparametrize the torsion strengths. Further work is ongoing for optimization of the GROMOS-53A6 force field. Generic modules and programs have been constructed as a part of the procedure, which can be reused for parametrization of other novel molecules.

LONI Support Role

Discuss and coordinate infrastructure upgrade for CCT, LI and LA-SiGMA

In LA-SiGMA charter, which is a result of efforts by LONI faculty for statewide initiatives for improving research merit, there is a strong push for moving to larger scale computational platforms ('supercomputing') and hybrid (GPGPU-CPU) architectures.

The LI scientist has been involved in active discussions with CCT and technology service staff across LONI campuses to upgrade equipment to HD quality. This will provide a leap in long distance teaching initiatives of LI. Two demos between LSU and LATech were carried out, in partnership with CISCO, LONI and BoR members, to test the viability. More demos are planned in future acquire suitable systems.

Coordinate with and support CCT staff for Materials World Focus Area (MWFA) long-distance classes, meetings and infrastructure upgrade

LI faculty at LSU are involved in teaching long distance courses in partnership with LATech, LSU, OSU, and ETH. Support for setup and test of H323, IOCOM and WEBEX based systems was provided with help from LI-CS A. Khaliq.

MWFA recently set a GPU computing lab in Johnston 244 with LI faculty M. Jarrell, R. Hall and J. Moreno. LI-CS Bhupender Thakur was actively involved in discussions and due-diligence efforts leading to purchase and set up about 10 GPU(GTX460) based workstations and 1GPU(M2070) server. Other efforts also included setting up a small library, printing and presentation area.

Coordinate and disseminate LI/LA-SiGMA seminar series

LI Scientist Bhupender Thakur was also responsible for coordinating LA-SiGMA seminar series for fall 2010. In spring 2011, the CS extended support to LI faculty D. Genov who was responsible for organizing the seminars. Efforts for seminars ranged from inviting nominations and selecting speakers to managing dissemination of the talks on Access Grid to all partner LONI and LA-SiGMA sites. With help from other LONI scientists, the LI scientist helped provide the necessary logistics. A brief description of the talks is provided on the seminar webpage http://institute.loni.org/li-lasigma-series.php

Support for Outreach efforts at LSU and LI

LI-CS participated in Nano world organized by LI faculty. The LI-CS is also leading weekly discussions of the GPU group. During the summer it will involve defining projects for some LA-SiGMA REU students. Over a longer term, it involves defining projects for MS and Ph.D. students.

Panels and discussions for human resource hiring

LI-CS was involved in panel interviews for hiring a Masters graduate student, currently being supervised by him, and ongoing efforts for hiring another LI scientist at LSU.

Seminars And Workshops

Supercomputing Nov 2010
LA-SiGMA kick off Meeting Aug 2010
4th LBRN Workshop on Computational Biology
LA-SIGMA All Hands Meeting May 2011

Dr. Shizhong Yang, SUBR

Research Group Members:
Graduate students --- Lei Zhao, Jialin Lei, Rui Yao, Rui Guo, Corey Baham, Vani Panguluri (just graduated this past Spring 2011); Undergraduate: Yalin Liu

Research Interests
Computational method development, computational materials and biochemistry

Roles and Specializations
Group leader, dedicated areas are computational simulation and experimental verification

Research Projects

Large-Scale First Principles Computation and Simulation of Catalytic Properties of Nitrogen Doped Carbon Nanotubes for Dioxygen Reduction

Role: Co-PI, HPC coding and performance test, model setup, data analysis, and mentor of graduate students
Collaborator: Dr. Guang-Lin Zhao (PI, Physics Department, SUBR), Dr. Ebrahim Khosravi (Co-PI, CMPS, SUBR)
Graduate Students: Lei Zhao, Jialin Lei, and Rui Guo.

Project Description:
We propose to perform first principles density functional calculations for the catalytic properties of nitrogen doped carbon nanotubes (CNTs) for dioxygen reduction. We aim to understand, (i) the stable structure of nitrogen doped CNTs; and (ii) the electronic and catalytic properties of the N-doped CNTs for dioxygen adsorption and reduction.

Precious platinum (Pt) catalyst is a key ingredient in fuel cells, which produce electricity and water as the only byproduct from hydrogen fuel. However, platinum is rare and expensive. Reducing the amount of Pt loading by identifying new catalysts is one of the major targets in the current research for the large-scale commercialization of fuel cells. Specifically, developing alternative catalysts to substitute platinum for the oxygen reduction reaction (ORR) in the fuel cell cathodes is essential, because the slow kinetics of this reaction causes significant efficiency losses in the fuel cells. Recent intensive research efforts in reducing or replacing Pt-based electrode in fuel cells have led to the development of new ORR electrocatalysts, including carbon nanotube–supported metal particles.

In 2006, Ozkan and coworkers reported that nitrogen-containing nanostructured carbons and nanotubes have promising catalytic activity towards ORR. In a 2008 report, Yang *et al.* at Argonne Laboratory showed that the vertically-aligned carbon nanotube (CNT) arrays, which are functionalized through nitrogen and iron doping by a chemical vapor deposition (CVD) process, can be electrocatalytically active

toward ORR. They further identified FeN_4 sites, which are incorporated into the grapheme layers of aligned carbon nanotubes, being electrocatalytic active.

In a 2009 publication in *Science*, Gong *et al*. reported that vertically aligned nitrogen-containing carbon nanotubes (VA-NCNTs) can act as a metal-free electrode with a much better electrocatalytic activity, long-term operation stability, and tolerance to crossover effect than platinum for oxygen reduction in alkaline fuel cells. The functionalized CNTs show promise properties as an alternative non-Pt electrocatalyst with a unique nano-architecture and advantageous material properties for the cathode of polymer electrolyte membrane fuel cell (PEMFC). They also performed hybrid density functional theory (DFT) calculations for the hydrogen edge-saturated (5, 5) CNT, in which a nitrogen atom doped in the middle of the nanotube. However, according to our recent *ab initio* simulation, nitrogen atoms prefer to stay at the open-edge sites of single wall (10, 0) CNT.

In order to understand the fundamental mechanism of the catalytic properties of the N doped CNTs for O_2 reduction, we need to perform chemical reaction path simulations. The PI, Khosravi, and Yang will perform the reaction barrier simulations using the Vienna Ab-initio Simulation Package (VASP), Q-Chem package (which is a recent developed quantum chemistry fast software package), and some supplemental data processing codes developed at SU HPC group. We had tested the exchange-correlation interaction potentials of the many electron system both in local density approximation (LDA) and in the generalized gradient approximation (GGA) with the same model and same parameters and found that they give the consistent results in the stability studies of nitrogen doped CNTs. We will develop an efficient and reliable model for structure optimizations. The calculated results from the two software packages will be compared carefully for verification of the calculated catalytic properties of nitrogen doped CNTs for dioxygen reduction reaction. We expect that the reduced-reaction-barrier quantity for dioxygen reduction reaction on nitrogen doped CNTs can be calculated. All the simulation will be performed on LONI machines.

One computational barrier for this proposed work is that the need of a large number of variable coordinates during the minimal energy path(MEP) search. We will test the reasonable coordinate number and then perform the simulation based on MEP algorithm. The experimental verification part will be performed in LSU CAMD in collaboration with professor Eizi Morikawa's group.

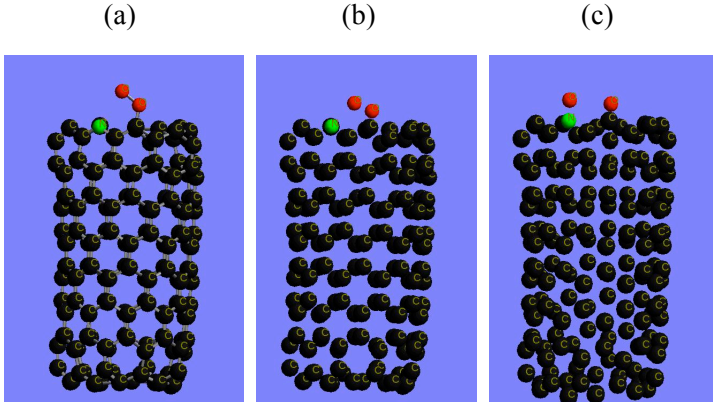


Figure 1. Snapshot of the simulation results from our accepted book chapter: (a) Side view of the initial state of dioxygen O_2 adsorbed onto a nitrogen-carbon complex site of the short CNT (Pauling model). The red balls stand for oxygen atoms, green ball stands for N atom, while black are C atoms. (b) Side view of the transition state of dioxygen/NCNT adsorption. (c). Side view of the dissociated two O atoms adsorption on the edge carbon and N atoms of the short CNT.

The proposed project will lead a fundamental understanding of the novel non-precious-metal catalysts. One graduate student will be involved in the project. The success of the project will also increase the future success in acquiring DOE funding support.

A novel *ab initio* molecular dynamics method for Cr-Y high temperature alloy simulation

Role: PI

Collaborators: Co-PIs: Ebrahim Khosravi (Computer Science, Southern University), Shengmin Guo (Mechanical Engineering Department, Louisiana State University)

Graduate students: Lei Zhao, Jialin Lei, Rui Guo, Corey Baham, and Rui Yao.

Project Description:

Introduction**:** This project will support two current DOE projects, lead by Drs. Yang and Guo respectively (award No. DE-FE0004734, $199,596, June 2010 ~ May 2012, and award No. DE-FE0003693, $500,000, Oct. 2010 ~ Sept. 2013) and in collaboration with NETL Principal Material Scientist M. Gao in high temperature alloy simulation research. The goal of this project is to develop reliable interatomic potentials from the highly accurate *ab initio* molecular dynamics (MD) calculation for Cr-Y system. Clean coal power generation is critical for the United State economic growth and international competitiveness. The key component for advanced coal power generation is a durable high temperature alloy. Chromium(Cr), a refractory metal, based high temperature alloys show considerable promise due to their relative low cost, low density, and good high temperature strength. We will use the developed interatomic potential to optimize the Cr-Y composition and processing environment through enhanced high temperature microstructures, melting points, elastic constants, diffusion coefficients, activation energy, and oxidation and sulfate corrosion resistance simulations. Dr. Yang and graduate students will develop the potential generating codes, perform property test, and develop HPC MD code and perform simulation on LONI HPC machines.

Proposed research

In this project, we will integrate *ab initio* calculations with MD simulations to enhance capabilities for materials modeling and prediction. As is well known, an appropriate potential of the interatomic interaction is the key to the success of the MD simulations. Unfortunately, not much data is available for complex materials. Ideally, a microscopic theory of quantum calculation that can produce such a potential would be very beneficial. Therefore we will utilize *ab initio* quantum computations to provide the input information of the interatomic potentials that will be used in MD simulations. The resulting computer codes will have the capability of MD calculations with the reliability of the *ab initio* method. We will develop the interatomic potentials for Cr, Y, and Cr-Y. Then the NVT ensemble will be chosen to simulate the high temperature elastic constants and diffusion coefficients and activation energy. The typical NVT MD run will be about 30,000 MD step with t=0.002 ps for the simulation. The small size test jobs, to test the parameter settings, will be performed on our workstations. After the scalable code tests, the HPC high temperature molecular dynamics simulation will be performed on Louisiana Optical Network Initiative (LONI) and TeraGrid supercomputers.

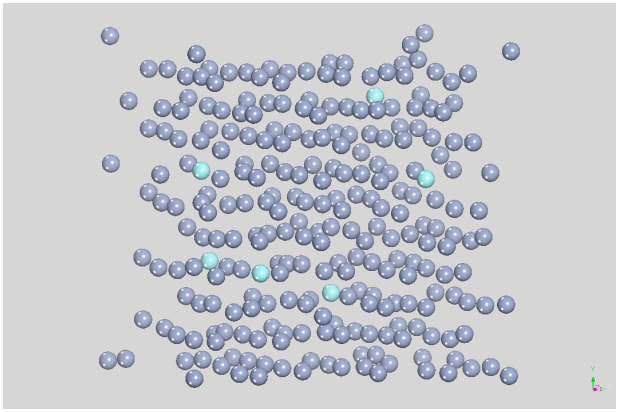


Figure 2. Cr-Y (244:6, 2.5%) MD simulation results on LONI machine at 2000K with 1.5 ns.

Broader impact

The proposed project will develop a novel ab initio MD simulation method and perform test on the Cr-Y alloy using LONI HPC facilities. The project will enhance our current collaboration with LSU and NETL lab to perform advanced research. Currently, Dr. Yang's group has six graduate students and one

undergraduate student working on a variety of funded projects. The proposed project will train under-represented minority students in high performance computing. Its outcomes have the potential to lead to long-lasting research, educational, and outreach efforts, which will reach far beyond the proposal period. Successful implementing the proposal will lead to secure more funding from DOE and NASA with potential big impacts to material science and especially for gas turbine industry.

Molecular dynamics simulation of the interactions of apocynin, 5-Nitroapocynin, and diapocynin with 1K4U subsection of human neutrophil NADPH oxidase system

Role: Co-PI

Collaborators: Rao M. Uppu PI, Environmental Toxicology, Southern University, Ebrahim Khosravi, Computer Science, Southern University

Project Description

This project is supported by funding from NSF SBIR IIa program of NCRR [grant number IIP-0956877, $505,014, 12/1/2010-3/31/2012]. Apocynin (Apo) is a potent phenolic antioxidant isolated from plants belonging to the apocyanaceae family. Apo has long been recognized for its potential to treat inflammatory and degenerative conditions. It is generally believed that Apo inhibits the plasma membrane NADPH oxidase system by interfering with translocation of key cytosolic components $p40^{phox}$, $p47^{phox}$ and $p67^{phox}$. In order to gain an insight into the nature of ligand- binding sites, we performed flexible docking of Apo and DiApo with 1K4U subsection of NADPH oxidase system using ICM-Pro (Molsoft) software. The study also included docking of 5- nitroapocynin (5-NitroApo), a nitration product known to be formed in reactions of Apo with nitric oxide-derived oxidants namely peroxynitrite and its CO_2 adducts. We have finished the ICM docking simulation and find the possible docking sites. The molecular dynamic simulations are needed to detail the atomic level interactions of Apo and its metabolites with $p47^{phox}$ and $p67^{phox}$ subunits of the NADPH oxidase system. We propose **three months** of Dr. Yang's research time to set up models, build force field, perform HPC simulation, and analyze the results, interactions and properties.

Proposed research

Plasma membrane NADPH oxidase of phagocytic cells is a multi-component system consisting of three cytosolic proteins ($p47^{phox}$ and $p67^{phox}$, and $p40^{phox}$) that translocate from the cytosol to the flavocytochrome in the plasma membrane upon stimulation of the cells. The enzyme system is the major source of superoxide anion which subsequently is converted to much stronger oxidants as hypohalous acids and peroxynitrite. While these oxidants play a pivotal role in bactericidal and fungicidal activities of phagocytic cells, the same oxidants can induce inflammation and oxidative stress in surrounding cells and tissues. Often, it is regarded as a kind of collateral damage that superoxide-producing cells need to incur in addition to their own loss due to oxidant-induced apotototic and/or necrotic cell death. Apocynin, a naturally-occurring phenolic antioxidant has long been known for its anti-inflammatory properties. The underlying mechanism(s) of apocynin and/or its metabolites inhibiting NADPH oxidase system has not been elucidated yet. We have shown that apocynin can also undergo nitration in the peroxynitrite/CO_2 reactions and form 5-nitroapocynin, and the possible crystal structure of 5-nitroapocynin has also been elucidated. Herein we attempt to simulate the interactions of apocynin, diapocynin and 5-nitroapocynin of the $p47^{phox}$ subsection (PDB: 1K4U) of NADPH oxidase system using NAMD software and analysis tools plus Yang's group's property calculation codes. Dr. Yang will setup the model and force fields, perform HPC MD simulation on LONI machines, and calculate, analyze, and compare the three types of systems.

Broader impact

The proposed project will build up the three types of force field for the MD simulation and calculate the interactions and properties of the three systems with intensive use of LONI HPC facilities. Currently, Dr. Uppu has a post doc and a Ph. D. student working on the experimental part of the research. Dr. Yang has six graduate students and one undergraduate student working on his projects. The proposed project will

train under-represented minority students in high performance computing. Its outcomes have the potential to lead to long-lasting research, educational, and outreach efforts, which will reach far beyond the proposal period. We believe successfully implement the project would lead to further NSF/NIH funding support.

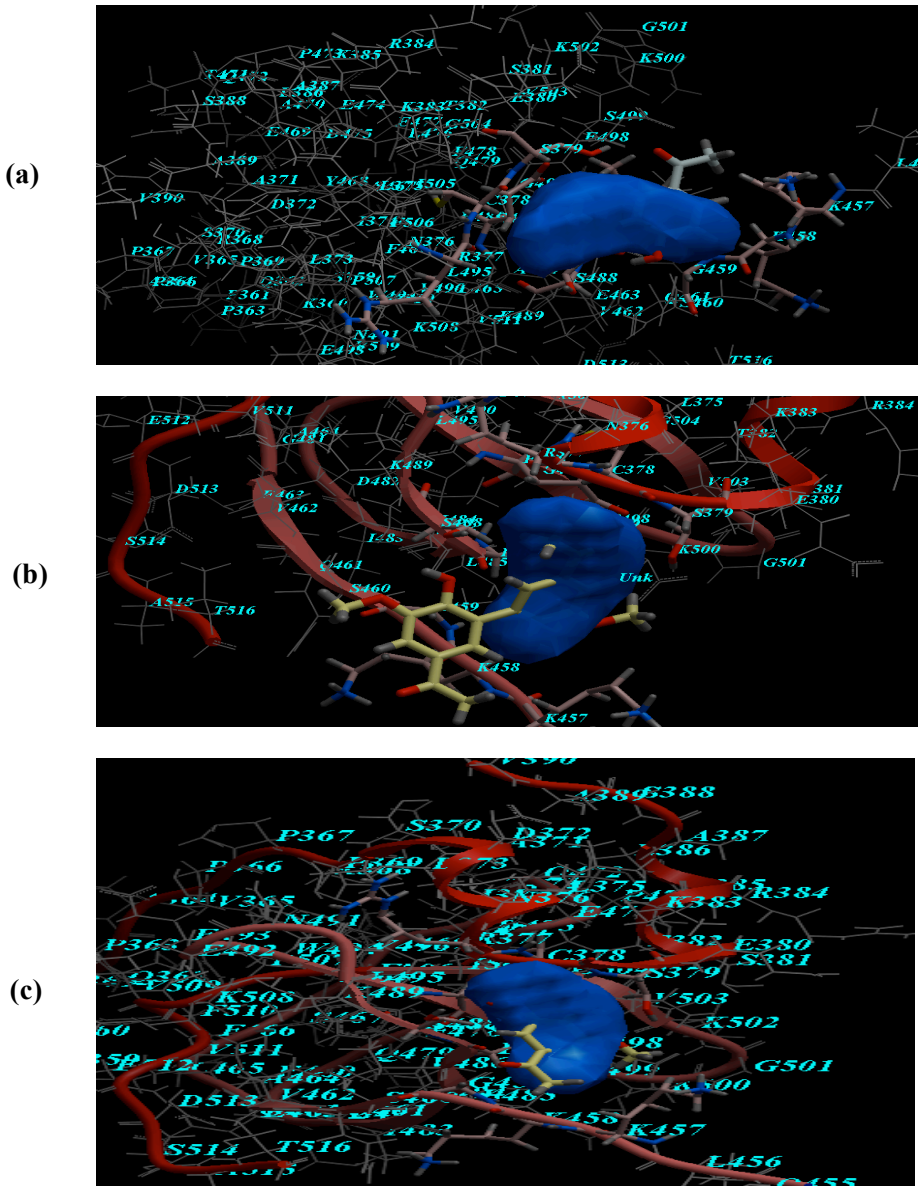


Figure 3: ICM docking of ligands: (a) apocynin; (b) diapocynin; and (c) 5-nitroapocynin on 1K4U ($p47^{phox}$/$p67^{phox}$). Three pockets are available in the 1K4U subsection for binding. The docking shown is in pocket 3 near Cys378. The MD simulations confirmed the above three structures are stable structures. (Graph from Vani Panguluri's thesis for submitting to journal publication)

Publications (07/01/10 - 06/30/11)

- Shizhong Yang, Guang-Lin Zhao, and Ebrahim Khosravi First principles studies of nitrogen doped carbon nanotubes for dioxygen reduction Journal of Physical Chemistry C **114** 3371 (2010).
- Shizhong Yang, Shengmin Guo, Shuju Bai, Ebrahim Khosravi, Guang-Lin Zhao, and Diola Bagayoko, Doped C60 study from first principles simulation, Journal of superconductivity and novel magnetism **23** 877 (2010).
- Shizhong Yang, Guang-Lin Zhao, and James M. Phillips, The electronic structures of commensurate Ru(0001)-(3 × 3) -4Kr and Ru(0001)- (5 × 5)-Kr using density functional theory, Surface Science **604** 1102 (2010).
- Wenyan Yin, Daniel V. Esposito, Shizhong Yang, Chaoying Ni, Jingguang G. Chen, Guanglin Zhao, Zhengjun Zhang, Changwen Hu, Minhua Cao and Bingqing Wei, Controlling Novel Red-Light Emissions by Doping In_2O_3 nano/Microstructures with Interstitial Nitrogen, Journal of Physical Chemistry C **114** 13234 (2010).
- Shizhong Yang, Guang-Lin Zhao, and Ebrahim Khosravi, Dioxygen adsorption and dissociation on nitrogen doped carbon nanotubes from first principles simulation, in printing, Carbon Nanotube, InTech, 2011.

Presentations / Talks (07/01/10 - 06/30/11)

- Invited Talk, NETL Albany Lab (joint with Pittsburg/Morgan Town and three local Universities), June 2, 2011, "*Ab Initio* DFT and molecular dynamics simulation on high temperature materials".
- Invited talk, 8th New3SC conference, "Computer simulation on the $AxFe_2Se_2$ high temperature structure superconductor", June 8~11, 2011, Beijing.
- LAS 85 Annual meeting, Electronic structure and optical properties of a Ta doped yettria-stabilized tetragonal zirconia from ab initio simulation, Lei Zhao, Goldie Jordan, Shizhong Yang, Ebrahim Khosravi, and Shengmin Guo, Feb. 26, 2011, Monroe, LA.
- LAS 85 Annual meeting, *Ab initio* study of copper atoms/cellulose segments interaction, Jialin Lei, Shizhong Yang, Ebrahim Khosravi, and Kun Lian, Feb. 26, 2011, Monroe, LA.
- APS March Meeting, "dissociation on nitrogen doped carbon nanotubes (10, 0) from first principles simulation", Shizhong Yang , Guang-Lin Zhao , Ebrahim Khosravi Dallas, TX, March 2011.

External Funding (07/01/10 - 06/30/11)

Funded:

- Title: Computer Simulation and Experimental Validation on the Oxidation and Sulfate Corrosion Resistance of Novel Chromium Based High Temperature Alloys (PI: S. Yang, Co-PI: E. Khosravi)
  Source of Support: DOE
  Award Amount (or Annual Rate): $__199,596_____
  Period Covered: 7/1/2010--6/30/2012
  Location of Activity: SU-BR, LSU-BR
- Title: Novel Nano-Structured Thermal Barrier Coatings (PI: S. M. Guo, Co-I: S. Acharya, M. Wahab, S. Yang, P. Mensah, R. Diwan)
  Source of Support: NASA-EPSCoR
  Award Amount (or Annual Rate): $__1,416,000
  Period Covered: 10/1/2009--9/30/2012
  Location of Activity: LSU-BR, SU-BR

- Title: Computational Design and Experimental Validation of New Thermal Barrier Systems (PI: S. Guo, Co-PI: E. Khosravi and S. Yang)
  Source of Support: DOE
  Award Amount (or Annual Rate): $____500,000_____
  Period Covered:__10/01/2010-- 9/30/2013_____
  Location of Activity: SU-BR

Submitted:

- Title: MRI: Acquisition of A High Performance Computing Cluster for Integrated Research (PI: E. Khosravi, Co-PI: S. Washington, N. Gwee, G.L. Zhao, and S. Yang)
  Source of Support: NSF
  Award Amount (or Annual Rate): $____1,867,989
  Period Covered: 9/15/2010 -- 9/14/2013
  Location of Activity: SU-BR
- Title: CDI-Type II: Predictive Quantum Computation of the Electrocatalytic Properties of New Catalysts for Green Energy Applications (PI: G.L. Zhao, Co-PI: J. Chen and S. Yang)
  Source of Support: NSF
  Award Amount (or Annual Rate): $____1,082,412
  Period Covered:__10/01/2010-- 9/30/2013_____
  Location of Activity: SU-BR, LSU-BR

Pending:

- (1). Title: High Temperature Sensors for in Situ Monitoring and Control of Gas Turbine Engine (PI: S. Guo, Co-PI: S. Acharya, D. E. Nikitopoulos, P. J. Schilling, S. Yang, E. Khosravi, and G. Zhao)
  Source of Support: DOE
  Award Amount (or Annual Rate): $____5,475,543____
  Period Covered:__10/01/2011-- 9/30/2014_____
  Location of Activity: LSU-BR, SU-BR

Education and Outreach (07/01/10 - 06/30/11)

- **Mentoring of graduate and undergraduate students in the Computer Science and at SUBR:** graduate students --- Lei Zhao, Jialin Lei, Rui Yao, Rui Guo, Corey Baham, Vani Panguluri (just graduated this past Spring 2011); undergraduate: Yalin Liu).
- **Mentoring the CMPS 592: Advanced Topic in Computer Science.** 12 graduate students used LONI machines to compile and test the performance of current DFT and MD codes.

Misc. (07/01/10 - 06/30/11)

1. **Hosts of the LI/LA-SiGMA seminars:**
   - 9/30/2010: Diola Bagayoko, "A Mathematical Solution to the Theoretical Underestimation of Energy and Band Gaps and Applications to the Search of Novel Materials", Moore Hall 218, SUBR.
   - 10/21/2010: Michael Gao, NETL Albany Lab, "Developing High-Temperature Alloys for Fossil Energy Applications", Moore Hall 218, SUBR.
2. **Invited talk/performing experiment at national labs and international conference:**
   - Invited Talk, NETL Albany Lab (joint with Pittsburg/Morgan Town and three local Universities), June 2, 2011, "*Ab Initio* DFT and molecular dynamics simulation on high temperature materials".
   - LBNL beamline 12.2.2, performing high pressure Cr-Y X-Ray axial experiment up to 42 GPa, May 22 ~ May 26, 2011.

- Invited talk, 8th New3SC conference, "Computer simulation on the $AxFe_2Se_2$ high temperature structure superconductor", June 8~11, 2011, Beijing.

Dr. Zhiyu Zhao, UNO

Research Interests
Bioinformatics algorithms and applications; parallel and distributed algorithms and applications

Research Projects

1. Isoform Level Human Transcriptome Identification using RNA-seq

Role: Co-PI, algorithm designer, software developer, and mentor of graduate students
Collaborator: Dr. Dongxiao Zhu (PI, Department of Computer Science, UNO)
Graduate Students: Kristen Johnson (master student, Department of Computer Science, UNO), Tin Nguyen (PhD student, Department of Computer Science, UNO)

Description:

The goal of this project is to develop a computational infrastructure with a Graphical User Interface (GUI) for identification of context-specific human transcriptome at the isoform level and to make it freely available for biomedical researchers to substantially accelerate the disease transcriptome research. Next generation sequencing (NGS) has provided unprecedented opportunities to *de novo* identify transcript structures and quantify transcript abundance at the isoform level. Despite improvements in sequencing methods and bioinformatics advances allowing *de novo* construction of transcriptoms, the existing approaches are often not sufficient to detect certain transcripts.

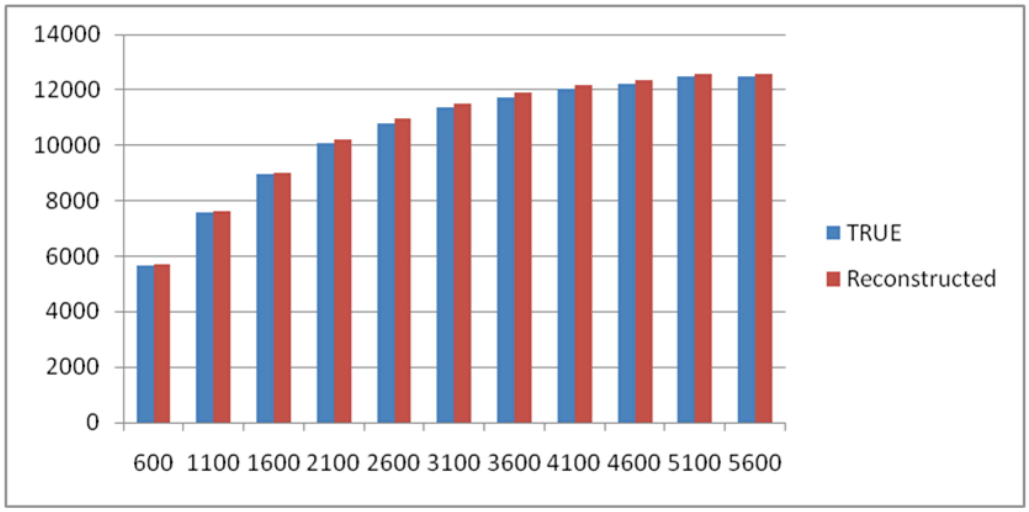
We propose a new statistical model to explain how the observed base-wise coverage signal is accumulated from a mixture of sibling isoforms. When the gene expression abundance is unknown, we propose a new constrained optimization algorithm to estimate isoform proportion and gene expression level simultaneously. Thus the real challenge comes in the computational side in that our iterative algorithm must be applied to a total of 22,000 genes annotated in the human genome. The problem size makes it necessary for us to develop an efficient parallel algorithm and run it on a powerful supercomputer such as those available on the LONI clusters.

This project will benefit LONI by fostering collaborative efforts from Louisiana institutions in their efforts in multidisciplinary human health related research. The proposed computational infrastructure is quite general and widely applicable to diverse human disease tissues wherever the RNA-seq data is available. Therefore, the proposed computational systems will benefit a wide range of researchers at large. This work also fits well the goals of the state as a whole -- Louisiana is investigating significant resources in growing the biotechnology industry. Long-term, expansion in this area may interest the biotech/pharmaceutical industry and tie in with statewide emphasis on biotech.

Tasks that have been accomplished or are ongoing include: (1) A *de novo* transcriptome assembly and isoform reconstruction algorithm has been designed to solve the proposed research problem. (2) A MATLAB prototype program has been developed to implement the algorithm. (3) Whole transcriptome-wise simulation data have been generated and used to test the performance of the algorithm. More tests are ongoing. (4) The algorithm is being improved to process data with sequencing errors. (4) A Java GUI is being developed to facilitate the use of this tool by interested researchers. The tool is going to be

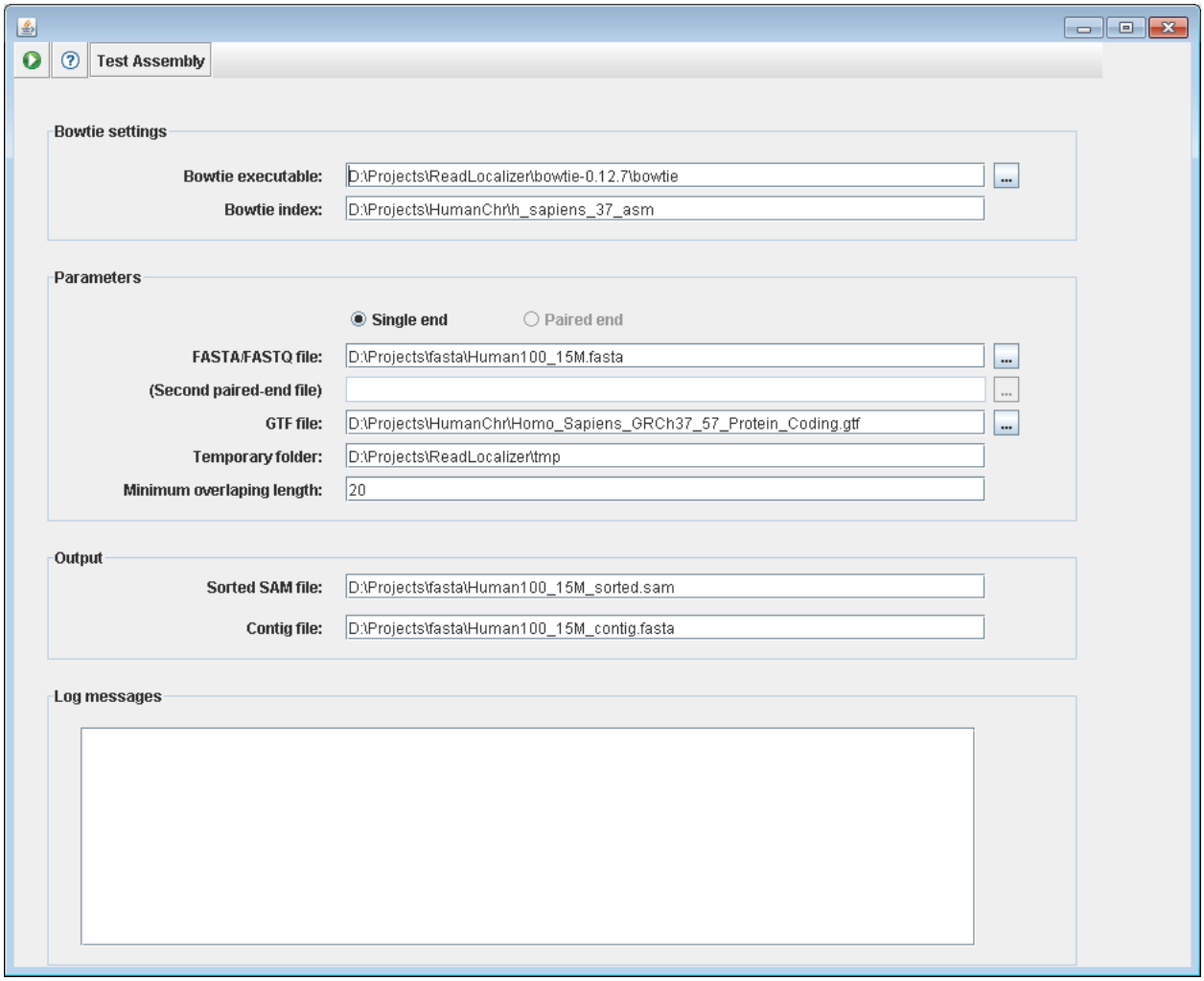
published and made free for download. (5) The MATLAB program has been rewritten in Java and incorporated into the Java GUI.

We use simulated NGS short reads to assess the accuracy of our proposed algorithm. We compared two independent sets of sequence contigs, one is given by the ground truth (a subset of the annotated transcripts), and another is reconstructed using our proposed algorithm. Our comparisons are concerning the total counts of contigs in each set and the amount of overlaps between two sets of contigs. In the figure below, horizontal axis represents the sizes of contigs and vertical axis represents the counts of contigs at each given size range. It is observed that the two sets of contigs have a very similar length distribution. In terms of base-wise coverage, for the data of 15 million reads, 93.4% of the bases in the ground truth contigs were covered by the reconstructed contigs, while 98.7% of bases in the reconstructed contigs were covered by the ground truth contigs.



TRUE vs. Reconstructed: 93.4%; Reconstructed vs. TRUE: 98.7%

Below is a snapshot of the Java tool being developed by Tin Nguyen:



2. Improving Antibody Design by Structure Prediction: Comparison of Computational and Molecular Approaches

Role: Co-PI, methodology designer, software developer, and experiments designer
Collaborators: Dr. Seth Pincus (Research Institute for Children, Children's Hospital New Orleans & LSU-HSC), Dr. Grace Maresh (Research Institute for Children, Children's Hospital New Orleans & LSU-HSC), Dr. David Worthylake (Department of Biochemistry and Molecular Biology, LSU-HSC)

Description:

This research addresses the design of high affinity Abs, which can be used as therapies for human disease, in biodetectors and diagnostics, or as a well-characterized model for general protein design. The project studies a monoclonal Ab that neutralizes the toxin ricin, a molecule of biodefense concern. Although it is already an effective Ab, we postulate that it can be made better by rational design (other projects in the lab are taking more "random" combinatorial approaches).

Computational Approaches
Dr. Zhiyu Zhao has developed a primitive computational tool which combines homemade programs with publically available resources to allow for computational tasks such as CDR loops identification of Abs, sequence search, structure search, structure alignment, Ab structure modeling, Ab-Ag docking and

binding energy estimation. Using this tool, she has been predicting the 3-D structure of the anti-ricin Ab, RAC18, and the complex structure of RAC18 binding to ricin A chain. She has also been using her sequence and structure search programs to find proteins structurally similar to RAC18 and docking them with the known structure of ricin to predict sites of contact, and how protein-protein interactions may be improved to produce higher binding affinity. Once the real structures of RAC18 and the Ab-ricin complex are determined, we will compare computational models with real structures and determine the accuracy of different models. Knowing the real structures will allow refinement of structure prediction and docking models.

Biological Experiments

Bioinformatics and computational biology are closely related fields that are undergoing a rapid expansion. Unfortunately, the number of people able to understand the complexities of both biomedicine and computer science are limited. It is our belief that the best way to attain expertise of this sort is to expose computer scientists to the rigors of molecular biology, bioassays, and analysis of such data. Over the past year, Dr. Zhao has learned a variety of immunological and biochemical techniques and been able to produce, purify, and characterize monoclonal Abs. She has also designed experimental protocols to allow our lab assistants to produce sufficient Abs for use. The next stage of the project is to screen for crystallization conditions. These studies are being performed in the laboratory of Dr. Worthylake, a crystallographer at LSUHSC-NO. Complexes of Ab-ricin are being made in high concentration. High throughput screens, using the hanging drop method in microwells, have been used to establish optimal crystallization conditions. With the identification of these optimal conditions, large scale crystallization is being performed in Dr. Worthylake's lab. If sufficient high quality crystals are obtained, then X-Ray diffraction studies will be performed.

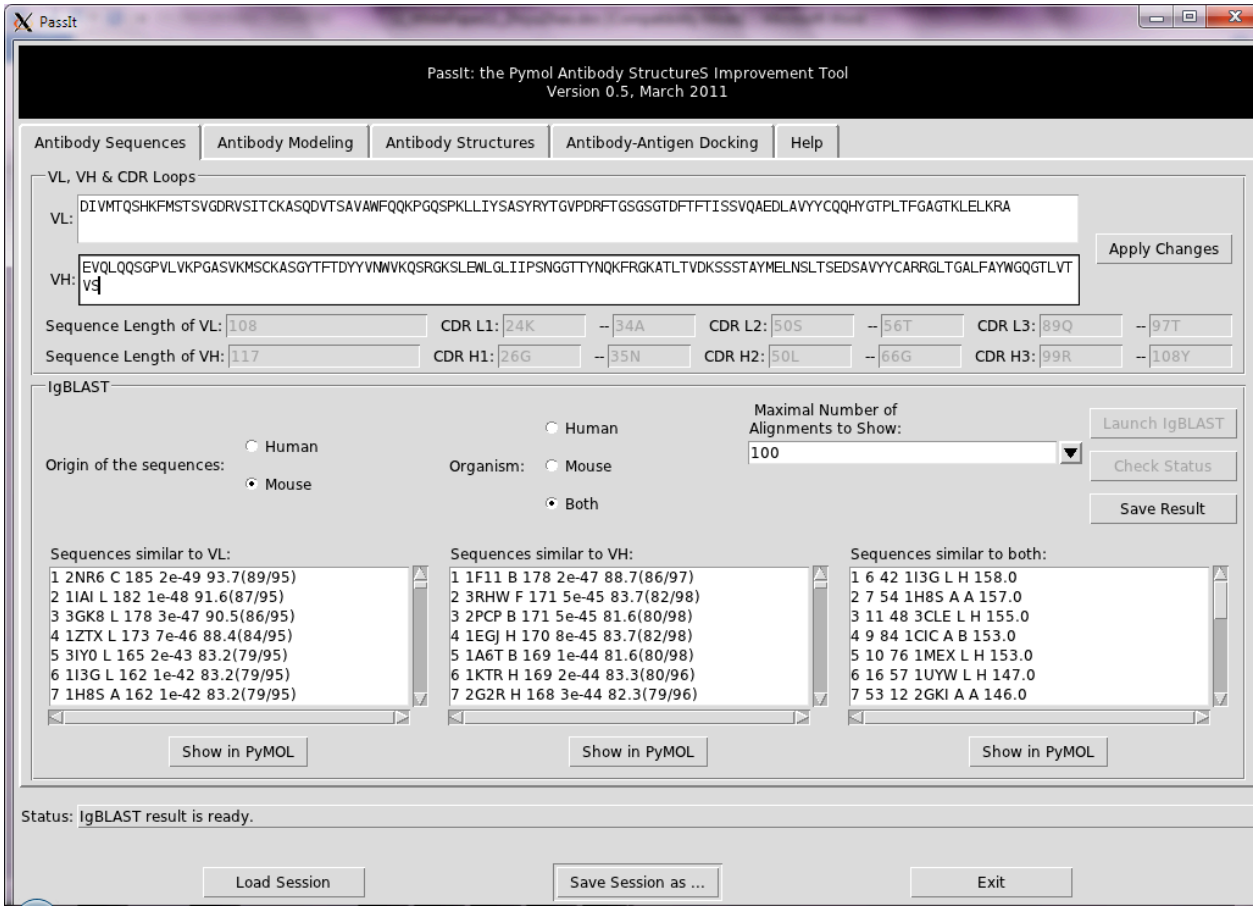
Long-term goals

Once the 3-D structure of the Ab binding to ricin is obtained, we will compare the results with those from computational modeling. Because Ab is such a well-studied molecule, the chance for informative results is high. These results can be used to refine existing computational models for the 3-D structure and antigen binding interfaces of Abs. The next step is to use this 3-D model to computationally predict amino acid changes that will produce a higher-affinity interaction between Ab and ricin. These changes can then be designed, synthetic genes made, and mutant Ab produced and tested for biological function. The ability to rationally improve Ab binding to Ag is a highly sought goal, and can be generalized to the improvement of other protein-protein interactions.

Benefits to the LI

Besides its importance in improving antibody design, this interdisciplinary and inter-institutional research proposal well meets the merits of LI. The project will broaden the scientific impact of LI in the participating institutions, has great potential to attract external funding support, and the developed computational tools will benefit researchers who are interested in designing novel proteins for efficient interactions. We have been regularly broadcasting a joint bioinformatics seminar with UNO's bioinformatics faculty via the Access Grid.

Below is a snapshot of the Python tool being developed by Zhiyu Zhao:



Publications (07/01/10 - 06/30/11)

- Huimin Chen, Zhiyu Zhao, Kun Zhang and Dongxiao Zhu, "New Aspects of Haplotype Inference from SNP Fragments", *A Practical Guide to Bioinformatics Analysis*, 173-183 (iConcept Press, Australia), June 2010.
- Liang Ding, Bin Fu, Yunhui Fu, Zaixin Lu and Zhiyu Zhao, "O((log n)^2) Time Online Approximation Schemes for Bin Packing and Subset Sum Problems", the Fourth International Frontiers of Algorithmics Workshop (FAW'2010, China), August 2010.
- Xu G, Deng N, Zhao, Z, Flemington EK, Zhu D. (2011) SAMMate: A GUI tool for processing short read alignment information in SAM/BAM format. *Source Code for Biology and Medicine*, 6(1):2, January 2011.
- Deng N, Puetter, A, Zhang, K, Johnson, K., Zhao, Z, Taylor, C, Flemington, E and Zhu, D., Isoform-level microRNA-155 Target Prediction using RNA-seq. *Nuc. Acid Res.*, 39(9): e61, May 2011.

Presentations / Talks (07/01/10 - 06/30/11)

- 08/23/10: "A Computational Method for Improving Antibody Structures", Research and Education Building, Children's Hospital, New Orleans; a presentation to bioinformatics faculty and graduate students at the University of New Orleans and the Research Institute for Children, Children's Hospital New Orleans.

- 04/12/11: “MATLAB – A Language and IDE for Scientific Computing”, NCF Annex, Xavier University of Louisiana, New Orleans; a tutorial to undergraduate students in the Department of Computer Science at XULA.

External Funding (07/01/10 - 06/30/11)

1. **Project 1**

- D. Zhu, "Computational Approaches for miRNA Target Prediction.", Xavier University, New Orleans, 08/10, 1 year, $24,456.
- D. Zhu, "MicroRNA Target Prediction Using RNA-seq.", Ladies Leukemia League Grant, 08/10, 8 months, $15,000.
- D. Zhu, "Graduate Student Services Agreement (Thair Judeh and Tin Nguyen).", Research Institute for Children, New Orleans, 08/10, 1year, $29,948.
- D. Zhu, "Human Transcriptome Quantification and GUI Software Development", LONI, 08/10, 1 year, $24,467.

Dongxiao Zhu’s PhD student, Guorong, Xu, was granted this 1-year graduate fellowship by LONI.

- D. Zhu, "Biomarker Discovery for Lung Diseases Using High Throughput Data.", Tulane Health Science Center, 07/10, 1 year, $24,456.
- D. Zhu, "An Informatics Paradigm for Reconstructing Signaling Pathways in Human Diseases.", NIH/NLM, 09/09, 2 years, $409,531.
- D. Zhu, "MicroRNA Target Prediction Using RNA-seq.", Tulane Cancer Center, 08/09, 1 year, $20,000.
- D. Zhu, "Analysis of Epstein Barr Virus type III Latency on Cellular miRNA Gene expression", Tulane Health Sciences Center, 06/09, 15 months, $137,638.
- D. Zhu et al, "NIH/NLM summer research supplemental request for R21LM010137-01.", funded by NIH/NML, 06/10, 1 year, $90,292.

Zhiyu Zhao is a co-PI of this grant.

2. **Project 2**

- Research Institute for Children, Children’s Hospital New Orleans: travel support, Fall 2010
- Zhiyu Zhao was granted travel support and registration fees to attend the Biotechnology and Bioinformatics Symposium (BIOT-2010), Lafayette, Oct 14 – 15, Louisiana.
- NIH grant AI059376, Children’s Hospital (a student stipend and supplies for biological experiments), and the Louisiana Vaccine Center.
- Dr. Worthylake is the recipient of NIH grant GM084072, and was the prior recipient of an RCS grant from Louisiana Board of Regents.

Teaching (07/01/10 - 06/30/11)

1. **Mentoring of graduate and undergraduate students in the Computer Science and Electrical Engineering departments at UNO on LI projects:**
   - Kristen Johnson: undergraduate student, Department of Computer Science, summer 2010 - present.
   - Tin Nguyen Chi: Ph. D. student, Department of Computer Science, fall 2010 – present.
   - Peiran Xu: undergraduate student, Department of Electrical Engineering, summer 2010 - present.
2. **Computer Science undergraduate courses at UNO:**
   - Fall 2010: CSCI 2467 (System Programming Concepts, 3 credit hours), CSCI 3080 (Ethics in Computing Profession, 1 credit hour) and CSCI 3090 (Undergraduate Seminar, 1 credit hour)
   - Spring 2011: CSCI 2125 (Data Structures and Algorithms, 3 credit hours), CSCI 3080 (Ethics in Computing Profession, 1 credit hour) and CSCI 3090 (Undergraduate Seminar, 1 credit hour)

Misc. (07/01/10 - 06/30/11)

1. **Papers in preparation:**
   - Zhiyu Zhao et al, "A *de novo* transcriptome assembly and isoform structure identification algorithm".
   - Zhiyu Zhao et al, "A parallel change point analysis algorithm for the detection of DNA copy number variations".

2. **Submitted proposal:**
   - D. Zhu et al, "Gene Modeling of Structural Variations using RNA-seq", an R-21 proposal submitted to NIH.

   Zhiyu Zhao is a co-PI of this proposal.

3. **Coordination of the LI/LA-SiGMA seminar series:**
   - 11/18/2010: Sandeep Patel, "Recent Progress in Development And Application Of Non-Additive Interaction Models For Molecular Simulations Of Biophysical And Physicochemical Systems", Science Building 2049, UNO
   - 4/26/11: Jake Chen, "Computational drug discovery using translational bioinformatics tools", Science Building 2049, UNO
   - 6/1/2011: Valeri Petkov, "Nanostructure by high-energy XRD and atomic pair distribution functions", Science Building 2049, UNO

2010 LI Graduate Fellows

Mr. Murat Seckin Ayhan, Center for Advanced Computer Studies (CACS), ULL

Advisor: Dr. Vijay Raghavan

Research Project

Below is a brief of our journal paper to appear in the BIBM 2010 Special Issue of International Journal of Data Mining and Bioinformatics (IJDMB).

Alzheimer's disease (AD) is one major cause of dementia. Previous studies have indicated that the use of features derived from Positron Emission Tomography (PET) scans lead to more accurate and earlier diagnosis of AD, compared to the traditional approaches that use a combination of clinical assessments. In this study, we compare Naive Bayes (NB) with variations of Support Vector Machines (SVMs) for the automatic diagnosis of AD. 3D Stereotactic Surface Projection (3D-SSP) is utilized to extract features from PET scans. This stereotactic approach provides both statistical analysis and standardization of PET imagery so that an objective, data-driven analysis is accomplished. At the most detailed level, the dimensionality of the feature space is very high. Hence we evaluate the benefits of a correlation-based feature selection method to find a small number of highly relevant features.

The feature selection procedure is beneficial for both NB and SVM in the sense that it dramatically reduces the dimensionality. We further show that the improvement in classification accuracy obtained for

NB is statistically significant. However, the feature selection technique leads to slightly lower performance accuracy for SVMs investigated; this may be due to the importance for the SVM approach of retaining correlated features. Hence, we suggest that a feature selection strategy, which could exploit strong attribute interactions, be adopted for SVMs.

We also provide an analysis of selected features, which is generally supportive of the literature. One supportive example stems from the posterior cingulate cortex, which resides on a major pathway in limbic system and is deemed to characterize early-to-moderate AD. The pathway is known as Papez circuit and its involvement in memory is crucial. In this respect, features from posterior cingulate cortex are greatly favored, due to their correlations with the degree of disease. On the other hand, primary motor, sensory and visual cortices remain functioning normal until very severe stages of AD. Consequently, these cortical regions were expected to be less preferable to the feature selection procedure. The pons region, which referred to for normalization purposes, is also spared by AD, which is analogous to the occipital association and visual cortices. In this respect, we are surprised that the pons region is favored by CFS because it seems contradictive to what we have observed with occipital association and visual cortices. A similar pattern is also observed with primary sensorimotor cortex. These findings are potentially indicative of new and relevant patterns regarding the prediction of the progression of AD, which requires further collaboration with domain experts, such as neurologists and radiologists, by which we hope to close the gap between our analysis and medical literature.

Peer-reviewed journal publications

- M.S. Ayhan, R.G. Benton, V.V. Raghavan, S. Choubey and ADNI (2011) *Exploitation of 3D Stereotactic Surface Projection for Predictive Modeling of Alzheimer's Disease*, International Journal of Data Mining and Bioinformatics BIBM 2010 Special Issue (*to appear*)

Peer-reviewed conference proceedings/presentations

- M.S. Ayhan, R.G. Benton, V.V. Raghavan and S. Choubey (2010) *Exploitation of 3D Stereotactic Surface Projection for Automated Classification of Alzheimer's Disease according to Dementia Levels,* IEEE International Conference on Bioinformatics and Medicine (IEEE BIBM 2010), December 18-21, 2010, Hong Kong, SAR, China (invited for submission to International Journal of Data Mining and Bioinformatics)
- M.S. Ayhan, R.G. Benton, V.V. Raghavan and S. Choubey (2010) *Determining Relevant Features based on 3D Stereotactic Surface Projection to Detect Dementia Caused by Alzheimer's Disease,* The 7th Annual Biotechnology and Bioinformatics Symposium (BIOT-2010), October 14-15, 2010, Lafayette, LA, USA (extended abstract)

Presentations

- I made a presentation for our paper entitled "Exploitation of 3D Stereotactic Surface Projection for Automated Classification of Alzheimer's Disease according to Dementia Levels" at IEEE International Conference on Bioinformatics & Biomedicine in Hong Kong during December 18-21, 2010. I had also given another talk on the same topic at the 7th Annual Biotechnology and Bioinformatics Symposium (BIOT-2010) in Lafayette, LA during October 14-15, 2010.
- Dr. Ryan G. Benton also gave a public presentation, title of which was "Towards Computer-Aided Diagnosis of Alzheimer's Disease", to the members of IEEE Lafayette Section on January 27, 2011. This talk included results and discussions from various papers published by our group members and various collaborators.

Patent or licensing agreements
Our studies constituted a joint effort between GE Healthcare and UL Lafayette. In the scope of the Early Health Collaboration project led by Dr. Vijay Raghavan, I developed a software prototype that demonstrates the machine learning for Alzheimer's disease. This software is GE proprietary. Delivery was completed in December 2009 (before LI Graduate Fellowship). It also included a user manual and documentation for the software. Following the prototype delivery, I delved into exploratory aspects of computerized diagnosis of AD.

LONI and the HPC resources
In regards to LONI resources and environment, I attended LONI workshops and tutorials. I implemented a correlation-based feature selection algorithm, which we utilized in our research. However, this implementation was not sufficient by itself for our advanced experimental setups. Thus, we used WEKA Data Mining software. We also figured out how to utilize WEKA tools in a parallelized manner; however, this requires a database management system (DBMS) available to users so that each remote experiment uploads its result to a shared database. Unfortunately, on the basis of my communication with LONI admins, it turned out that the DMBS within LONI is meant for administrative purposes, such as user account management. In this regard, in the future, LONI should try to make available of database to users. Especially, considering the popularity and capability of WEKA packages, it shall be beneficial for a wide range of researchers.

Collaborations
During the workshop, which was held in November 2010, I had my chances to communicate and consult with experts/tutors from LONI. I also attended the HPC tutorials via Access Grid.

Other Achievements
- IEEE BIBM 2010 Student Travel Award
- University of Louisiana at Lafayette Student Government Association (SGA) Travel Funding Award to attend IEEE BIBM 2010
- University of Louisiana at Lafayette Graduate Student Organization (GSO) Travel Funding Award to attend IEEE BIBM 2010

We acknowledged the LONI and LI Graduate Fellowship in our journal paper. Louisiana Board of Regents was also mentioned in the acknowledgement section. See below:

"The LONI Institute is an initiative funded by the Louisiana Board of Regents and six member institutions; Louisiana State University, Louisiana Tech University, Tulane University, Southern University, University of Louisiana at Lafayette, and University of New Orleans. I, Murat Seckin Ayhan, hereby, acknowledge the LONI Institute Fellowship award during the 2010-2011 academic year."

"This work was also partially supported by the Louisiana Board of Regents, via a Traditional Enhancement Grant (LEQSF(2009-10)-ENH-TR-67) entitled "Web 3.0 and Beyond: Enhancement of the Laboratory for Internet Computing for the Future Web Generation", which provided part of the computational infrastructure utilized in this study."

IEEE-CS Student Paper Contest, 3rd prize (slightly before the LI Graduate Fellowship)

M.S.Ayhan, (2010) A Comparative and Exploratory Brain Data Mining on Alzheimer's Disease Data, Center for Advanced Computer Studies, UL Lafayette, April 2010, USA

Mr. Shravan Rakesh Animilli, Department of Physics, LA Tech
Advisor: Dr. Dentcho A. Genov

Research Project

Surface Plasmon Enhanced Solar Cells (SPESC)

The principal objective of this project is to develop a highly efficient solar cell by integrating active plasmonic (metal-dielectric composites) media with the existing technology. The random metal-dielectric composites facilitate surface plasmon resonance (usually in optical and infrared regimes) with giant enhancement in the local electromagnetic (EM) fields. Utilizing these properties in the design of SPESC is expected to improve current yield through high photon-exciton conversion efficiencies. However, the design and optimization of SPESC requires memory intense and long run time calculations for computing the local EM fields of large number of strongly interacting metal nanoparticles. For instance a random system with one million metal nanoparticles particles requires 1-10 Tbits of shared memory and can take many years on contemporary workstations. We develop a new numerical techniques for solving the EM response of the composite medium. Our approach is based on solving the discrete current conservation (Kirchhoff's Equations) using the bond model. The Kirchhoff's equations are system of linear equations written through Kirchhoff Hamiltonian (KH) ($\widehat{\mathbf{H}}\mathbf{\Phi} = \mathbf{F}$) involving the local potentials and external field. We used MPI libraries (SCALAPACK), specifically the parallel subroutines *PCGBSV*, which we integrated with a partition of the Kirchoffs Hamiltonian for better memory management. Our method is based on elimination of a set of related banded matrixes, by dividing each matrix into blocks that are eliminated using *PCGBSV*. We employ SPMD (single process and multiple data) technique for the computation management under a distributed environment, we parallelized the BE method by integrating the memory partition subroutines (MPI commands). As we have a random system, parallelization is done based on the number of realizations such that each processor runs the BE method for one or more realizations independently. A run time output from the parallel code is depicted in Fig. 1, showing rather good scaling with the number of cores. We have already integrated our EM results within a separate model of SPESC optical and IV response. Our result show that enhancement in the overall solar cell efficiency of 67% can be achieved. Furthermore, to study effect due to exciton quenching at the metal substrate we are in the process of developing a 3D parallel code that will solve the SP eigenproblem, providing the complete density of states of the system which will be incorporated in the SPESC IV model in near future (Fall 2011).

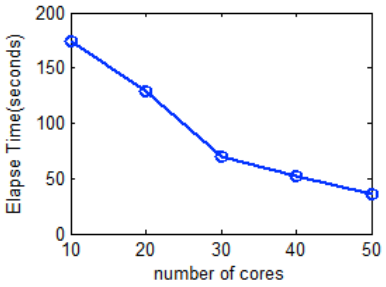


Figure: Time scaling for the parallel three dimensional BE code**.** Tested on Bluedawg super computer for system encompassing 400,00 metal particles.

Presentations

Desimone, D. G., M. A. Koorie, A. Thapa, S. R. Animilli, S. Zivanovic, and D. A. Genov, "Theoretical and experimental study of metal-dielectric composite electrodes for polymer solar cell enhancement", *Louisiana Academy of Sciences 85th Annual Meeting*, Monroe, LA, February 26 (2011).

LONI and the HPC resources

As these calculations require very large computational memory storage and high operational speed, the utilization of the HPC provided by LONI was crucial for this process. We have utilized both Bluedawg and Azul supercomputers, located at Louisiana Tech University.

Collaborations
Dr. Abdelkader Baggag provided a valuable input in the initial stages of this project and specifically with the MPI implementation of the SCALAPACK subroutines.

Mr. Corey Baham, Department of Computer Science, SUBR

Advisor: Dr. Shizhong Yang

Research Project
My research is titled, "Molecular simulation of a segment of gK protein" and is an extension of previous work by last year's graduate fellow Kimberly Lyles. I have studied the gk protein, its membrane, and its atomic structure. Also, I have used VMD and NAMD to perform simulations using input files created with the assistance of Dr. Shizhong Yang. The Protein Data Bank files, which are five times larger than the previous files, are almost complete. Thus, this work will be finished and presented as a thesis in mid-July. Prior research simulated a portion of the gk protein found in the Herpes Simplex Type-1 virus. After observing the membrane at 300 Kelvin at 100,000 time steps, the membrane appeared to have curled inward significantly, coming very close to the protein, almost to the point where new bonds could be formed. My findings focus on the protein chain that connects the prior research to the upper chain that also travels through the membrane.

Presentations
A public presentation of my work will soon be displayed in the Computer Science department of Southern University.

LONI and the HPC resources
I have used HPC resources, particularly machines Louie and Lacumba, to run jobs.

Collaborations
Dr. Shizhong Yang creates the protein data bank files needed for the simulations. Dr. Rachel Vincent-Finley provides guidance as well.

Mr. Lide Duan, Department od Electrical and Computer Engineering, LSU

Advisor: Dr. Lu Peng

Research Project
Universal Rules Guided Design Parameter Selection for Soft Error Resilient Processors
This work aims at characterizing and improving soft error reliability at the *pre-silicon* stage, i.e. before the processor is manufactured. Specifically, we correlate a processor's Architectural Vulnerability Factor (i.e. AVF, an important metric that quantifies soft error vulnerability for a computer system at computer architecture level) with a large processor design space, from which certain design parameter ranges are quantified to minimize the resulting configurations' AVF and thereby achieve soft error resilient designs.
In this work, I proposed to use a statistical rule search strategy named *Patient Rule Induction Method (PRIM)* to identify the design configurations with maximized soft error robustness. By efficiently exploring the processor design space, PRIM can generate a set of selective rules on key design parameters. Applying these rules at early design stage effectively identifies the design space subregion within which the output variable (i.e. AVF in this work) is considerably smaller than its average value over the entire design space. Therefore, the processor configurations selected by the generated rules are *inherently* reliable to soft errors. By utilizing this technique, I quantitatively demonstrated that (1)

minimizing the AVF for different processor structures may degrade or improve performance; and (2) reducing the AVF of a single structure may increase the AVF of others. Hence, a holistic reliability optimization achieving reasonable tradeoff with performance is necessary. This approach is further applied to multiprocessors running multi-threaded workloads. In order to simultaneously balance reliability, performance, and power for a multiprocessor, an objective function that achieves a good tradeoff among these conflicting metrics was proposed and examined.
Different from traditional application-specific design space studies, which build a separate model for each program, our PRIM model is *universal* for different programs. In other words, only a single model is trained, and the effectiveness of the generated rules is validated on programs not used in training. This cross-program capability provides model scalability in the era of multithreading.

Peer-reviewed conference proceedings/presentations
L. Duan, Y. Zhang, B. Li, and L. Peng, "Universal Rules Guided Design Parameter Selection for Soft Error Resilient Processors," in Proceedings of *IEEE International Symposium on Performance Analysis of Systems and Software (ISPASS)*, Apr. 2011.

Presentations
Lide Duan, "Universal Rules Guided Design Parameter Selection for Soft Error Resilient Processors," Conference Presentation at *IEEE International Symposium on Performance Analysis of Systems and Software (ISPASS)*, Austin, TX, Apr. 2011.

LONI and the HPC resources
My research work is based on statistical methods, thus requiring an extremely large number of software simulations to obtain statistically reliable results. I submitted my simulation works to LONI clusters (e.g. Queenbee). These results consumed more than 100K processor hours, and appeared in my publication listed above.

Other Achievements
Lide is currently working as a research intern in Lawrence Livermore National Laboratory (LLNL) in Livermore, CA. He will support the development of error propagation models for numerical applications for the "Reliable High Performance Peta- and Exa-Scale Computing" project. Specifically, he will conduct fault injection experiments on numerical routines from the BLAS, LAPACK, and GSL libraries, analyze the results of these experiments, and train statistical models to represent the effects of errors on individual routines and compose the models of individual routines to create error propagation models of entire applications.

Mr. Elliott James, College of Engineering and Science, LA Tech
Former advisor: Dr. Abdelkader Baggag

Research Project
I worked with Dr. Ramu and Dr. Dai to develop numerical differentiation schemes for a Finite Difference Time Domain (FDTD) scheme that is used to solve the time-dependent Schrödinger equation. My initial proposed work, was related to parallel algebraic multigrid and its application to the three dimensional time-dependent Navier-Stokes equation, but this work was abandoned due to the unexpected and abrupt departure of my research advisor, Dr. Abdelkader Baggag in October of 2010. Under the supervision of Dr. Dai, I developed a hybrid MPI-GPU algorithm for analytically differentiating the Lagrange interpolating polynomials. This algorithm uses MPI to provide distributed shared memory (DSM) allowing the use of multiple physical machines and OpenCL to provide access to accelerators, which in this case are ATI 5870 graphic processing units (GPUs) and Nvidia Tesla 2050 GPUs. The code also

makes use of OpenMP, which enables each MPI process to take advantage of multicore CPUs, exploiting multiple levels of parallelism inside each machine and globally via MPI. While this algorithm is extremely efficient, with a sequential runtime of 460 days, a parallel runtime when using pure MPI of 22 days, and a hybrid MPI-GPU runtime of 1.5 days, we have been forced to abandon the underlying mathematics (and the algorithm), because of instabilities in the differentiated Lagrange interpolating polynomials.

Peer-reviewed journal publications
No publications at this time, due to the departure of Dr. Baggag, my agenda and research focus changed abruptly, I am targeting two Journal publications in Fall of 2011.

Presentations
Presented work done under Dr. Baggag at SCALA 2011 at Tulane University.

LONI and the HPC resources
I used LONI's HPC research for some initial test of my pure MPI code. Since LONI does not provide any hybrid clusters (clusters with GPUs or other Accelerators), I performed most of my work using resources provided by Dr. Chokchai (Box) Leagsuksun, as well as my own computing resources.

Collaborations
I worked with Dr. Ramu on portions of the project, and was lead primarily by Dr. Dai, who is a LA-SiGMA professor.

Mr. Derrick Goss, Department of Mechanical Engineering, SUBR

Advisor: Dr. Patrick Mensah

Research Project
My research involves the empirical development of heat transfer convection coefficients. There are literally countless applications of this information ranging from cooling of computer microprocessors to design of automobile engine cooling systems. In conducting this research, I will develop empirical correlations (equations) using the wind tunnel here at Southern University for various geometries beginning with flat plate, and evolving to more complex geometries, and potentially evolving to entire systems. This research would be greatly enhanced with the supercomputing resources that would be provided by LONI. This is because the experimental research would need to be verified and compared to empirical correlations already available today. These calculations are very straightforward on a small scale, but require intensive computational resources when expanded to very complex geometries, which is very lengthy to perform of standard desktop computers.

Ms. Jerina Pillert, Biomedical Engineering Department, Tulane

Advisor: Donald Gaver

Research Project
Our aim with this current study is to identify ventilation waveform parameters that optimize transport and ultimately contribute to the development of pulmonary ventilation strategies that decrease damage to the epithelial lining of the lungs. Our computational domain consists of a semi-infinite air bubble propagating through an airway occluded with liquid doped surfactant. Specifically, we have modeled the flow and

transport fields in the fluid region ahead of and surrounding the air-liquid interface in an oscillating flow regime.

Figure 1 depicts an example pulsatile flow/transport field with an inactive surfactant and the following parameter values: $Ca = 0.1, Pe_b = 10^2, Pe_s = 10^3, St_a = 10^5, St_d = 5 \times 10^4$. The capillary number ($Ca$) relates viscous to surface tension forces, the Peclet numbers (Pe_b and Pe_s) relate convection rates to diffusion rates in the bulk (b) and the interface (s), and the Stanton numbers (St_a and St_d) relates adsorption (a) and desorption (d) rates to surface convection rates.

These preliminary results indicate that the inclusion of oscillatory flow fields can significantly modify transport near the bubble tip potentially allowing for optimal surfactant transport and adsorption to the interface. This system will be further investigated by modifying the parameters described above. Currently, we are in the process of parallelizing and reducing the time of computation in order to increase our ability to analyze the system efficiently.

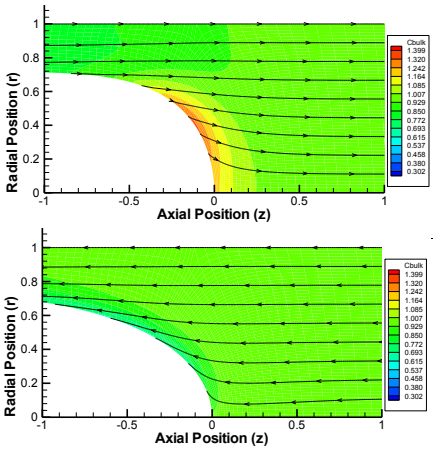


Figure 1: Preliminary results. The top graph illustrates a backward flow portion in the oscillation cycle while the bottom graph depicts forward flow.

We have shown that oscillations enhance surfactant transport and adsorption particularly in the backward flow portion of the flow cycle. With further investigation of this model we will assess the transport of surfactant and the effect of the adsorbed surfactant on interfacial shape and its influence on the mechanical stress field; particularly the normal-stress gradient that can damage epithelial cells in ventilator-induced lung injury (VILI).

Presentations

- Annual Biomedical Engineering Society Conference (Oct. 6-9th 2010). "A computational study of surfactant biophysical interactions during pulsatile airway reopening."
- SSE Research Day at Tulane University (April 7th 2011) "A computational investigation of surfactant transport during pulsatile airway reopening."
- Tulane Engineering Forum (April 15, 2011) "A computational investigation of surfactant transport during pulsatile airway reopening."

LONI and the HPC resources

I am just starting to use LONI resources. The code has been developed and tested on a desktop (workstation) and is now being parallelized and formatted to run on Louie and Queen Bee.

Collaborations

Hideki Fujioka, Ph.D. and LONI Institute Computational Scientist, Center for Computational Science, Tulane University.

Ms. Shanshan Shen, Mathematics Department, Tulane

Advisor: Ricardo Cortez

Research Project

My current research focuses on the blob projection method for immersed boundary problems in two-dimensional domain. The blob projection method is based on the idea that a cutoff function, or blob, is used to regularize the force field. Then the force field is computed directly on a regular Cartesian grid via a smoothed dipole potential. The blob projection method is based on the idea that a cutoff function, or blob, is used to regularize the force field. Then the force field is computed directly on a regular Cartesian grid via a smoothed dipole potential.

Here is what I have done:

- used the velocity field due to a point force in whole space to approximate the velocity field in periodic boundary, which can be saved as reference solution.
- for some fixed blob function, studied how the errors and convergence rates are related to δ/h. (δ-blob size, h-grid size)
- did experiments on blob functions of different smoothness and different moment conditions, studied how smoothness and moment conditions effect convergence rates.

LONI and the HPC resources

IBAMR method is used on HPC resources

Mr. Guorong Xu, Department of Computer Science, UNO

Advisor: Dongxiao Zhu

Research Project

During the past year, we have developed a GUI software pipeline for quantifying human transcriptome (whole set of mRNA transcripts) using the Next-generation sequencing (NGS) data. For efficiently processing NGS data, our GUI software SAMMate allows biomedical researchers to quickly process SAM/BAM files and is compatible with both single-end and paired-end sequencing technologies. SAMMate also automates some standard procedures in DNA-seq and RNA-seq data analysis. Using either standard or customized annotation files, SAMMate allows users to accurately calculate the short read coverage of genomic intervals. In particular, for RNA-seq data SAMMate can accurately calculate the gene expression abundance scores and transcript expression abundance scores for customized genomic intervals using short reads originating from both exons and exon-exon junctions. Furthermore, SAMMate can calculate a whole-genome signal map at base-wise resolution in a short time allowing researchers to solve an array of bioinformatics problems. Finally, SAMMate can export both a wiggle files for alignment visualization in the UCSC genome browser and an alignment statistics report.

With just a few mouse clicks, SAMMate will provide biomedical researchers easy access to important alignment information stored in SAM/BAM files. Our software is constantly updated and will greatly facilitate the downstream analysis of NGS data. Both the source code and the GUI executable are freely available under the GNU General Public License at http://sammate.sourceforge.net.

Peer-reviewed journal publications

- Xu,G, Deng, N, Zhao, Z, Zhang, K, Judeh, T, Flemington, EK and Zhu, D: SAMMate: A GUI tool for processing short read alignment information in SAM/BAM format. *Source Code for Biology and Medicine*, 2011; 6:2.

- Zheng, L, Xu G, Taylor C, Zhu D, Flemington EK. (2010) Analysis of EBV transcriptome using RNA-seq. *J. Virology*, doi:10.1128/JVI.01521-10.

Presentations
Poster presentation during the conference Biotechnology and Bioinformatics Symposium (BIOT-2010), October 14-15, 2010, Lafayette, Louisiana

Patent or licensing agreements
The source code and the GUI executable are freely available under the GNU General Public License.

LONI and the HPC resources
Our software is still under developing and now it can support Linux platform since SAMMate v2.6. We are planning to test its performance on LONI clusters this summer.

Collaborations
We have interaction with Dr. Zhao Zhiyu, LI CS.

Other Achievements
We have submitted another peer-review paper and it is under review:
Xu, G, Deng, N, Duan, Z, Zhao, Z and Zhu, D*. iQuant: A fast yet accurate GUI tool for isoform quantification using RNA-seq. Submitted

Mr. Hongtao Yu, Department of Chemistry, UNO
Advisor: Steven W. Rick

Research Project
Two projects are done with LONI and are being prepared for publication. The first project is an extension of our previous one. In our previous project, protein model cavities that can accommodate only single water molecules are constructed and their water hydration thermodynamics, in term of free energy, entropy, and enthalpy, are calculated with thermodynamic integration technique. All cavity residues in our previous study are neutral small organic molecules [1]. Our current project extends this study by introducing charged residues into the cavity systems. Free energy calculation indicated that, cavities with charged residues prefer to be occupied by water molecules as long as they can form one hydrogen bond with hydration water molecules. This hydration pattern is different from the neutral cavities, in which at least two hydrogen bonds are required. The more favorable hydration free energies for the charged cavities are predominantly dominated by the hydration enthalpies; the hydration entropies share a similar structure between the charged and neutral cavities. Our second project concerns the influence of internal hydration water molecules on the protein dynamics and flexibility. Proteins with hydration water molecules included and excluded from the interiors are simulated with Amber molecular dynamics simulation package. Four proteins are simulated, the BPTI, the HEWL, and the PHS and PHSV66E mutants of Staphylococcal Nuclease. The simulations have been completed and data are under analysis.

[1] H. Yu and S. W. Rick "Free Energy, Entropy, and Enthalpy of a Water Molecule in Various Protein Environments" *J. Phys. Chem. B* **114**, 11552—11560 (2010)

Presentations
H. Yu, and S. W. Rick, ''Waters in Protein Interior and Their Influences on Protein Dielectric Permittivity'', 66th Southwest and 62th Southeastern Meeting for the American Chemical Society, New Orleans, LA, November 30th – December 4th, 2010

LONI and the HPC resources
We use LONI IBM AIX cluster to perform the Molecular Dynamics simulations.

Ms. Ashley Zebrowski, Department of Computer Science, LSU

Advisor: Dr. Gabrielle Allen

Research Project
I have been engaged in multiple fronts of research. The Cactus-Spawner project has been a major focus, enabling Cactus simulation components to run on multiple machines in parallel. Although it is still a work in progress, initial findings have indicated that it improves the performance of Cactus simulations which are constrained by some components that traditionally are required to run serially. The speed increase is greatest when the data and simulation transfer requirements are small, and intelligently determining how to get the smallest possible required subset of data is an ongoing part of my research. There are also important questions in modeling simulation component costs in various ways, which act as an "intelligence" in determining when and where to spread simulation components across various infrastructure.
The BL-Octree project has been another Cactus-centric project. Cactus' adaptive mesh refinement driver Carpet has some algorithmically inefficient code which provides $O(N^2)$ scaling. This limits Carpet so that it can only scale to around 10,000 processors efficiently. My work on BL-octree has been to provide a non-trivial improvement over the current Carpet implementation, allowing Cactus' AMR driver to run on many tens or hundreds of thousands of cores. Although it is still under development, our work has been solid enough that we expect full results within the next two months.
Another project I have been working on is a gateway project for scientific simulations. I have a fully-working Python framework which provides access to simulation results and analysis functions, which works in any web browser.
Finally, I have been working on a scheduling paper, examining the ways Cactus schedules functions internally and comparing that to other scheduling approaches to find commonalities between them. I hope to eventually use some of this work on LONI/LSU HPC resources and on resources such as the OSG.

Peer-reviewed conference proceedings/presentations
My work on the BL-octree has been accepted at the International Conference on Parallel Computing ("ParCo") conference. My work on the Cactus-Spawner project is forming the core of my M.S. project defense, which will occur this summer. The gateway and scheduling papers will likely be published some time in the future.

Presentations
At SC2011 I presented a poster with my Cactus-Spawner results.

LONI and the HPC resources
I used Queen Bee, Eric, and other resources to execute Cactus simulations. In addition, I also ran experiments with SAGA and Cactus-Spawner across multiple resources simultaneously to develop distributed functionality for Cactus.

Collaborations
I have worked with Erik Schnetter and Peter Diener on Cactus-Spawner. I have worked with Frank Loeffler and Erik Schnetter on BL-Octree.

Mr. Haochun Zhang, Mathematics Department, ULL
Advisor: Dr. Baker Kearfott

Research Project

My research involves developing branch and bound based optimization algorithms and that lend well to parallelization and have several applications in disaster management. I have been currently working on constructing a multi-objective optimization model to solve the problem of distributing relief supplies (through Points of Distributions) under various constraints. The objectives include maximizing the convenience (in terms of prepositioning the distribution points in close proximity to people), assessing the need (considering factors such as the Human Development Index, Social Vulnerability and purchasing power) and minimizing the distribution cost. The objectives in this model include minimizing cost, maximizing convenience and meeting demand. We consider a local optimization algorithm to find a single good and practical solution, then work to find all global solutions, that is, the Pareto frontier. Considering the huge amount of data for a particular geographical area, we will use parallel processing to implement our algorithm on LONI systems.

In this project, we have three levels, from easy to complicated, from local single good solution to all global optimal solutions. These are as follows:

(a) Develop a basic double-objective linear optimization model to describe our problem. In this case, the two objectives are minimizing cost and maximizing convenience. We will compare different definitions of convenience, to find the "best" ones for different types of disasters. In preliminary computations, we will pose the problem as a single-objective problem, considering one of the objectives as a constraint, which we can solve with linear programming technology.

(b) Develop a stochastic double-objective mixed model, to include random aspects of disaster. We will find an algorithm to solve this problem directly, so we can find all extreme effective points, the Pareto frontier.

(c) Implement a parallel branch and bound algorithm to solve our model from (2) based on the combination of MPI and Lpsolve (A linear programming library).

Branch and bound software for global optimization lends itself well to parallelization, since a search domain is divided into sub-domains, and each sub-domain can be processed more or less independently. Furthermore, there is a relatively large amount of processing on each sub-domain, so the ratio of computation to communication is high. Nonetheless, there are various issues, such as load-balancing, since each sub-domain generates additional sub-domains, and some sub-domains require more computation than others. Also, it is advantageous to share certain information, such as a sharper upper bound on a global minimum, soon after it is obtained. These issues have been studied by several groups, but have not been definitively resolved, especially in the case where mathematical rigor is required.

Peer-reviewed journal publications

We have been working on these two papers,

- **Zhang, H**, B. Kearfott, N. R. Gottumukkala, R. Kolluru, "Multi Objective Mixed Optimization model for Points of Distributions to distributed emergency supplies", 2011, to be submitted to the Transportation Research Part E: Logistics and Transportation Review.
- **Zhang, H**, B. Kearfott, N. R. Gottumukkala, R. Kolluru, "High-performance computing in Multi Objective Optimization problems", 2011, in process.

Peer-reviewed conference proceedings/presentations

- Presenter: Zhang, Haochun. Zhang, H, B. Kearfott, N. R. Gottumukkala, R. Kolluru, "Multi Objective Mixed Optimization model for Points of Distributions to distributed emergency supplies," 2011 INFORMS Annual Conference, Nov. 7-10, 2010, Austin, TX.

- Zhang, H, B. Kearfott, N. R. Gottumukkala, R. Kolluru, "Multi Objective Mixed Optimization model for Points of Distributions to distributed emergency supplies", 2011, to be submitted to the Transportation Research Part E: Logistics and Transportation Review.

LONI and the HPC resources

My main work with LONI is to implement optimization algorithms, and develop parallel computing by using HPC, I have been working on "QueenBee" for my course projects and have a working knowledge on LONI through some of the projects at National Incident Management Systems and Advanced Technologies (NIMSAT). Such as participation in three workshops on training in high-performance computing on LONI, especially on how to use MPI and OpenMP to implement parallel computing.

Collaborations

I work with Dr. Raju Gottumukkala, LI CS, from Center for Business & Information Technologies at ULL on the project "Fuel Demand Estimation for Regional Hurricane Evacuation".

LI Senior Investigators

Journal and conference publications

- NGUYEN, H. V., ORTIZ, R., CORTEZ, R., FAUCI, L. J. The action of waving cylindrical rings in a viscous fluid. *J. Fluid Mech.* V. 671, p.574-586 (2011)
- CORTEZ, R., CHRISPELL, J. C., KHISMATULLIN, D. B., FAUCI, L. J. Shape oscillations of a droplet in an Oldroyd-B fluid. *Physica D (2011), doi:10.1016/j.physd.2011.03.004*
- ARANDA, V., CORTEZ, R., FAUCI, L. Peristaltic pumping of a viscous fluid in a three-dimensional tube: a new twist, *Physics of Fluids*, accepted (May 2011).
- CORTEZ, R., NICHOLAS, M. Regularized Slender Body Theory. In review.
- Smith*, B.J., E. Yamaguchi and D.P. Gaver. A translating stage system for micro-PIV measurements surrounding the tip of a migrating semi-infinite bubble. Measurement Science and Technology, 21(1): 015401 (13pp), January 2010.
- Smith*, B.J., and D.P. Gaver. Agent-based computational simulations of droplet dynamics in a two-branch microfluidic network. Lab on Chip, DOI: 10.1039/b916380h, 2010.
- Zamir, M., J. E. Moore Jr., H. Fujioka, and D. P. Gaver, Biofluid mechanics of special organs and the issue of system control. Annals of Biomedical Engineering, 38(3): 1204-1215, March 2010.
- Glindmeyer* IV, W., B. Smith* and D. Gaver. Physicochemical enhancement of pulmonary surfactant using pulsatile ventilation. In Review.
- Halpern, D. and D.P. Gaver III. The influence of surfactant on the propagation of a semi-infinite bubble through a liquid filled compliant channel. In revision, J. Fluid Mech.
- Hamlington, K.L., H. Fujioka, R. Cortez and D. P. Gaver III. A parallel mesh-free algorithm to simulate high Péclet number convection-diffusion-reaction in irregular geometries. In Review
- Smith, B.J., S. Lukens, E. Yamaguchi and D.P. Gaver III. Lagrangian transport properties of pulmonary interfacial flows. In review
- R. Singh, J. Monk and F. R. Hung, "A computational study of the behavior of the ionic liquid $[BMIM^+][PF_6^-]$ confined inside multi-walled carbon nanotubes", *J. Phys. Chem. C* **114**, 15478-15485 (2010)
- J. Monk, R. Singh and F. R. Hung, "Effects of pore size and pore loading on the properties of ionic liquids confined inside nanoporous CMK-3 carbon materials", *J. Phys. Chem. C* **115**, 3034-3042 (2011)

- J. Chen, F. Ehrenhauser, T. P. Liyana-Arachchi, F. R. Hung, M. J. Wornat and K. T. Valsaraj, "Adsorption of gas-phase phenanthrene on atmospheric water and ice films", *Polycycl. Aromat. Comp.*, accepted (2011). Interinstitutional.
- R. Singh, J. Monk and F. R. Hung, "Heterogeneity in the dynamics of the ionic liquid [BMIM+][PF6-] confined in a slit nanopore", *J. Phys. Chem. C*, submitted (2011)
- T. P. Liyana-Arachchi, K. T. Valsaraj and F. R. Hung, "A molecular simulation study of the adsorption of naphthalene and ozone on atmospheric air/ice interfaces", *J. Phys. Chem. A*, submitted (2011).
- "Energy Landscape Analysis for Regulatory RNA Finding using Scalable Distributed Cyberinfrastructure" J. Kim, W. Huang, S. Maddineni, F. Aboul-ela, S. Jha, in press, Concurrency and Computation: Practice and Experience (2011).
- Y el-Khamra, H Kim, S Jha and M Parashar, Autonomic Management of Applications Workflows on Hybrid Computing Infrastructure, accepted for Scientific Programming, Special Issue on Science-driven Cloud Computing (2011)
- A Thota, A Luckow and S Jha, "Efficient Replica-Exchange Simulations on Large-Scale Production Grids", accepted for publication in the Philosophical Transactions of the Royal Society London A (2011)
- D Katz, Scott Callaghan, Robert Harknesse, Shantenu Jha, et al., "Science on the TeraGrid", accepted for Computational Methods in Science and Technology, in (2011)
- S Sehgal, A Merzky, M Erdelyim, S Jha, "Understanding Application Level Interoperability: Scaling-out MapReduce From High-Performance Grids to Web-Scale Resources", accepted for Future Generation Computing Systems (FGCS), 2010
- Using off-diagonal confinement as a cooling method, V. G. Rousseau, K. Hettiarachchilage, M. Jarrell, J. Moreno, and D. E. Sheehy, Phys. Rev. A 82, 063631 (2010).
- Porous Manganese Oxide Shell around Copper Nanoparticles, Nachal D. Subramanian, Juana Moreno, James J. Spivey and Challa S.S.R. Kumar, submitted to the Journal of Physical Chemistry Letters.
- Dynamical Cluster Approximation, H. Fotso, S. Yang, K. Chen, S. Pathak, J. Moreno, M. Jarrell, K. Mikelsons, E. Khatami, and D. Galanakis, Theoretical methods for Strongly Correlated Systems, Springer-Verlag (to be published).
- The response to dynamical modulation of the optical lattice for fermions in the Hubbard model, Zhaoxin Xu, Simone Chiesa, Shuxiang Yang, Shi-Quan Su, Daniel E. Sheehy, Juana Moreno, Richard T. Scalettar, and Mark Jarrell, preprint arXiv:1104.1739.
- Dual Fermion Dynamical Cluster Approach for Strongly Correlated Systems, S.-X. Yang, H. Fotso, H. Hafermann, K.-M. Tam, J. Moreno, T. Pruschke, and M. Jarrell, preprint arXiv:1104.3854.
- Role of the van Hove Singularity in the Quantum Criticality of the Hubbard Model, K.-S. Chen, S. Pathak, S.-X. Yang, S.-Q. Su, D. Galanakis, K. Mikelsons, M. Jarrell and J. Moreno, preprint arXiv:1104.3261.
- Kenway, D Wright, S Jha, "Towards High-throughput and High-Performance Computational Estimation of Binding Affinities for Patient Specific HIV-1 Protease Sequences'", accepted for publication, ACM Proceedings of TeraGrid 2011
- J Kim, S Maddineni, S Jha, "Building Gateways for Life-Science Applications using the Dynamic Application Runtime Environment (DARE) Framework'", accepted for publication, ACM Proceedings, TeraGrid 2011
- S. Ko, et al., "CFD Toolkit: A Cactus Computational Toolkit for Parallel Multi-Block CFD Applications", International Conference on Parallel Computing, Ghent (Belgium), Sept. 2011
- F Löffler, G Allen, W Benger, A Hutanu, S Jha and E Schnetter, "Using the TeraGrid to Teach Scientific Computing", accepted for publication, ACM Proceedings of TeraGrid 2011

- J Kim, S Maddineni, S Jha, "Characterizing Deep Sequencing Analytics Using BFAST: Towards a Scalable Distributed Architecture for Next-Generation Sequencing Data", accepted for Emerging Computational Methods in the Life Sciences 2011, workshop held in conjunction with HPDC-2011
- "Exploring Adaptation to Support Dynamic Applications on Hybrid Grids-Clouds Infrastructure", H. Kim, Y. el-Khamra, S. Jha and M. Parashar, Accepted, ACM *ScienceClouds* Workshop as part of HPDC 2010
- B. Jiang, A. Struthers, Z. Sun, Z. Feng, X. Zhao, K. Zhao, W. Dai, X. Zhou, M. E. Berens, and L. Zhang, Employing graphic programming unit technology, alternating direction implicit method and domain decomposition to speed up the numerical diffusion solver for the biomedical engineering research, accepted by International Journal for Numerical Methods in Biomedical Engineering.
- A. Khaliq, F. Jenkins, M. DeCoster, and W. Dai, A new 3D mass diffusion-reaction model in the neuromuscular junction, accepted by Journal of Computational Neuroscience.
  W. Dai and D. Y. Tzou, An accurate and stable numerical method for solving a micro heat transfer model in a 1D N-carrier system in spherical coordinates, accepted by ASME Journal of Heat Transfer.
- D. Liu, Y. Lvov, and W. Dai, Joint simulations of confined diffusion inside nanotubules, Journal of Computational and Theoretical Nanoscience, vol. 8, pp. 1-11, 2011.
- W. Dai, An improved compact finite difference scheme for solving an N-carrier system with Neumann boundary conditions, Numerical Methods for Partial Differential Equations, vol. 27, pp. 436-446, 2011.
  R. Nassar, X. Wu, M. Paun, W. Dai, and J. Palmer, A mathematical model characterizing the diffusion properties of microcapsules, Chemical Engineering Communications, vol. 198, pp. 33-45, 2011.
- D. Zhao and W. Dai, Accurate finite difference schemes for solving a 3D micro heat transfer model in an N-carrier system with Neumann boundary condition in spherical coordinates, Journal of Computational and Applied Mathematics, vol. 235, pp. 850-869, 2010.
- N.B. Idupulapati and D.S. Mainardi, "Quantum Chemical Modeling of Methanol Oxidation Mechanisms by Methanol Dehydrogenase Enzyme: Effect of Substitution of Calcium by Barium in the Active Site", ***J. Phys. Chem. A***, *114* (4): 1887–1896 (**2010**)
- G.K.P. Dathara and Mainardi D.S., "Kinetics of Hydrogen Desorption in $NaAlH_4$ and Ti-Containing $NaAlH_4$" ***J. Phys. Chem. C***, *114* (17): 8026–8031 (**2010**)
- Idupulapati, N.B. and D.S. Mainardi. "Methanol Electro-Oxidation by Methanol Dehydrogenase Enzymatic Catalyst: A Computational Study", in ***Theory and Experiment in Electrocatalysis,*** *Modern Aspects of Electrochemistry V.50*. P.B. Balbuena and V. Subramanian Eds. New York, Springer Science Publishers. (**2010**)
- "Structural Patterns in (GaAs)n clusters", Gennady L. Gutsev, Mogus D. Mochena, Bidhan C. Saha, Pedro Derosa, and Charles W. Bauschlicher, Jr. Journal of Computational and Theoretical Nanoscience V. 7 (1) 254-263 2010.
- B. Ramachandran, Purnima Kharidehal, Lawrence M. Pratt, Stewart Voit, Fabian N. Okeke, and Monique Ewan, "Computational Strategies for Reactions of Aggregated and Solvated Organolithium Carbenoids," J. Phys. Chem. A 114, 8423-8433 (2010).

Invited presentations

- CORTEZ, R. (Presenter & Author), Blackwell-Tapia Conference, "Simulation of flagellar motions using regularization methods," Mathematical Biosciences Institute, Columbus, OH. (November 2010).

- CORTEZ, R. (Presenter & Author), Cha-Cha Days Workshop, "An agent-based spatial model of mosquito behavior in West Nile Virus," College of Charleston, Charleston, SC. (September 2010).
- CORTEZ, R. (Presenter & Author), Individual and Collective Fluid Mechanics of Swimming Microorganisms, "Simulation of flagellar motions near a surface," University of Glasgow, Glasgow, Scotland. (July 2010).
- CORTEZ, R. (Presenter & Author), SIAM 2010 Annual Meeting, "Regularization Methods for Biological Fluid Flow Problems," Society for Industrial and Applied Mathematics, Pittsburgh, PA. (July 2010).
- CORTEZ, R. (Presenter & Author), SIAM 2010 Annual Meeting, "Regularized Slender Body Theory," Society for Industrial and Applied Mathematics, Pittsburgh, PA. (July 2010).
- CORTEZ, R. (Presenter & Author), Individual and Collective Dynamics in Active Suspensions Workshop, "A model of collective motion of self-propelled organisms based on regularized elements" Institut Henri Poincaré, Paris, France (June 9, 2011).
- Smith, B.J., E. Yamaguchi, D. Gaver III. Pulsatile flow for the prevention of atelectrauma-based ventilator-induced lung injury. Proceedings of the 16th US National Congress of Theoretical and Applied Mechanics, June 27 - July 2, 2010, State College, Pennsylvania, USA (Plenary)
- Gaver, D.P. Pulmonary Atelectrauma Mechanisms of Damage and Protection. Biomedical Engineering Distinguished Lecturer Series, University of California, Irvine. November 5, 2010. Irvine, CA
- F. R. Hung, "Structure and dynamics of ionic liquids confined in nanoporous carbons", October 2010, Department of Chemical and Biological Engineering, The University of Alabama (department seminar / national)
- F. R. Hung, "Structure and dynamics of ionic liquids confined in nanoporous carbons", September 2010, Dave C. Swalm School of Chemical Engineering, Mississippi State University (department seminar / national)
- S. Jha, Microsoft Faculty Summit, July 2011, Seattle
- S. Jha, Invited Participant, NSF Workshop on ``Software for Grand Challenges for Chemical Sciences", June 2011, Oxford, UK
- S. Jha, Microsoft Cloud Futures Workshop, June 2011, Seattle
- S. Jha, Invited Talk, TeraGrid/Blue Waters Symposium on Data-Intensive Analysis, Analytics, and Informatics, April 2011, Pittsburgh Supercomputing Center
- S. Jha, Invited Colloquium, SUNY Binghamton (NY), Spring 2012
- S. Jha, eSI Public Lecture, Edinburgh (November 2010)
- S. Jha, Invited Colloquium, Leibnitz Supercomputing Center, Munich (November 2010)
- S. Jha, Invited Talk, Grid Interoperability, Brussels, October 2010
- S. Jha, Invited Colloquium, Bioinformatics Group, Amsterdam Medical Centre, September 2010
- S. Jha, Invited Talk, Session on HPC-HTC Interoperabilty, EGI Technical Forum, Amsterdam 2010
- S. Jha, Invited Participant, NSF-DoE-Air Force Research Lab Workshop on Dynamic Data-driven Application Scenarios, Washington, August 2010
- S. Jha, Invited Colloquium, Department of Computer Science, University of Houston, July 2010
- S. Jha, Invited Panelist, ``Data Intensive Cyberinfrastructure for Life Sciences", Emerging Computational Methods for the Life Sciences Workshop (June 2010)
- S. Jha, Invited Colloquium Speaker, University of Potsdam (Berlin), May 2010
- Juana Moreno, New magnetic materials for spintronics, U.S.-Japan symposium "Connections – Bringing Together the Next Generation of Women Leaders in Science, Technology, Engineering and Mathematics, July 5-7, 2010, Saitama, Japan, International.

- Juana Moreno, New magnetic materials for spintronics, Aoyama Gakuin University and University of Tokyo, Japan, July 2010. National.
- Juana Moreno, The Astounding Center for Computation and Technology, Highland Road Park Observatory, Baton Rouge, August 13, 2010. Local.
- Juana Moreno, New magnetic materials for spintronics, 11/2010, Howard University, Local.
- Juana Moreno, New magnetic materials for spintronics, PIRE Conference 2011, Wuerzburg, Germany, January 7-9, 2011. International.
- Juana Moreno, Opportunities in Computational Materials Science, 03/2011, Timbuktu academy, Southern University, Local.
- Juana Moreno, New magnetic materials for spintronics, 04/2011, Southern University, local.
- Daniela Mainardi, "Thermodynamics and Kinetics of Hydrogen Storage Systems", Invited oral presentation during the NSF-funded Indo-US Workshop: Emerging Issues in Energy and Environment Security: Challenges and Research Opportunities, The Claridges SurajKund, Delhi NCR, India, Dec 12-15, 2010. Scope: International.
- Pedro Derosa, "Using Computer Simulation across Scales", Xavier University, August 16, 2010, Regional.
- B. Ramachandran, "Selective complexation of alkali metal ions using calix[4]arene-crown-6 ethers: A computational investigation," Mississippi College, Clinton, MS, 01/25/2011, Regional.
- "Towards Computer-Aided Diagnosis of Alzheimer's Disease", IEEE Lafayette Section, January 27, 2011, local presentation, Presenter: R. Benton

Proposals to national agencies

- FAUCI, LISA J (Principal), CORTEZ, RICARDO (Co-Principal), GAVER, DONALD P (Co-Principal), "RTG: Mathematical and Computational Biofluids," Sponsored by NSF, Federal, $1,535,353.00. (AWARDED). Multidisciplinary
- CORTEZ, RICARDO, MCMAHON, CHARLES P (Co-Principal), "MRI-R2: Acquisition of a cluster named Desire," Sponsored by National Science Foundation, Federal, $3,246,998.00. (2009 - Present). (DECLINED)
- CORTEZ, RICARDO, Bryant, R. (Principal), "MSRI-UP: MSRI's Undergraduate Program," Sponsored by NSF, Federal, $322,767.00. (July 1, 2008 - June 30, 2012). (AWARDED)
- FAUCI, LISA J (Principal), CORTEZ, RICARDO (Co-Principal), Dillon (Co-Principal), Shelley (Co-Principal), Zhang (Co-Principal), Teran (Co-Principal), "Focused Research Group: Collaborative Research: Dynamics of," Sponsored by NSF, Federal, $1,390,973.00. (July 2007 - June 2012). (AWARDED)
- CORTEZ, RICARDO (Principal), "Regularization Methods: New Theory, analysis and applications," Sponsored by NSF, Federal, $364,457.00. (2006 - 2010).(EXPIRED)
- CORTEZ, RICARDO (Co-Principal), GAVER, DONALD P (Co-Principal), BLAKE, DIANE A (Supporting), BISHOP, THOMAS CONNOR (Supporting), ASHBAUGH, HENRY SNYDER (Supporting), Khonsari (BoR), M. (Principal), "Research Infrastructure Improvement," Sponsored by NSF EPSCoR, Federal, $1,913,373.00. (October 1, 2007 - September 30, 2010). (EXPIRED). Multidisciplinary.
- GAVER, DONALD P, CORTEZ, RICARDO, JOHN, VIJAY T, NAVAR, LUIS GABRIEL, CLEMENTS, JOHN D, "IGERT: Bio-innovation through biomedical technology and device development.," Sponsored by NSF, Tulane University, $2,673,460.00. (June 1, 2011 - May 31, 2016). (Declined). Multidisciplinary.
- Gaver, D.P. "A Two-Color mu-PIV/LIF System to Measure Unsteady Two-Phase Flow and Surfactant Transport Relevant to the Lung," NSF CBET-1033619, $299,867, 1/11-12/13.
- GAVER, DONALD P, CORTEZ, RICARDO, JOHN, VIJAY T, NAVAR, LUIS GABRIEL, CLEMENTS, JOHN D, "IGERT: Bioinnovation through biomedical technology and device

development.," Sponsored by NSF, Tulane University, $2,964,663. (June 1, 2012 - May 31, 2017). (Submitted). Multidisciplinary.

- "The Science and Technology of Dispersants Relevant to Deep-Sea Oil Releases" (PI: Vijay John, Tulane University; F. R. Hung is a participant with 46 other faculty from LSU and other universities in the US); $299,997 (F. R. Hung's part); BP Exploration & Production, Inc. (Gulf of Mexico Research Initiative); to be submitted on June 2011 (submission pending). Interdisciplinary, interinstitutional.
- "Solidification of organic salts confined inside nanopores" (PI: F. R. Hung; co-PI: I. M. Warner); $355,050; National Science Foundation; submitted on March 2011 (pending)
- "Collaborative research: Experimental and computational design of imidazoles for CO2 capture" (collaboration with University of Alabama; PI: J. E. Bara; co-PIs: C. H. Turner and F. R. Hung); $384,658 (F. R. Hung's part: $142,818); National Science Foundation; submitted on March 2011 (pending). Interinstitutional.
- "Molecular modeling of ionic liquids confined inside nanoporous carbons and silicas" (PI: F. R. Hung); $785,622; Department of Energy Early Career Research Program; submitted on November 2010 (declined)
- "New Dispersed Phase Materials Enabled by a Class 2 Hydrophobin" (PI: P. S. Russo, co-PI: F. R. Hung), $400,000; National Science Foundation; submitted on October 2010 (declined)
- "Understanding the solidification of organic salts confined inside nanopores" (PI: F. R. Hung; co-PI: I. M. Warner); $366,450; National Science Foundation; submitted on September 2010 (declined)
- "CEMRI: LSU Center for Research on Functional Materials" (PI: J. Y. Chan; F. R. Hung was a participant with other 22 faculty from LSU and other universities in the US); $15,000,000 (total); National Science Foundation; submitted on September 2010 (declined). Interdisciplinary, interinstitutional.
- "CAREER: Molecular simulation of ionic liquids in diverse environments" (PI: F. R. Hung), $400,000; National Science Foundation; submitted on July 2010 (declined)
- "Biomedical Imaging using NanoGumbos" (PI: I. M. Warner; co-PI: F. R. Hung, S. Das, B. M. El-Zahab, K. G. Kousoulas, M. Li); $1,472,799; National Institutes of Health; submitted on July 2010 (declined)
- S. Jha, Co-PI NSF Cyber-Enabled Discovery and Innovation, "Mapping complex biomolecular reactions with large scale replica exchange simulations on national production cyberinfrastructure", $1.6M (2011-2014)
- S. Jha, PI, NSF Award OCI-1059635 to Support Participation in the UK EPSRC Research Theme (via e-Science Institute, Edinburgh) on "Dynamic Distributed Data-Intensive Programming Abstractions and Systems", ($50,000; 09/2010 - 08/2011)
- S. Jha, ASTA Award for support of Advanced Science Scenario on Ranger and Kraken.
- S. Jha, Co-PI NSF-ARI proposal, $1.99M,"BIPAS-Bifurcated Infrastructure Promoting the Advance of Science: Revitalizing LSU's Data Network Infrastructure" (OIA-0963375)
- Juana Moreno, Co-Pi: D. Browne, J. Garno, M. Jarrell, J. Ramanujam, D. E. Sheehy (Louisiana State University), and P. Derosa (Louisiana Tech University and Grambling State University). Status: Awarded. Submission date: 12/2010. Beginning date: 01/2011. Ending date: 12/2011. Amount requested: 7 million SUs. Amount awarded: 4 million SUs. Title of award: Quantum Monte Carlo Simulations Employing The Dynamical Cluster Approximation. Grantor: Louisiana Optical Network Initiative (LONI). Award number: loni_dca_10
- Rongying Jin, Co-Pi: Julia Y Chan, Mark S. Jarrell, E. Ward Plummer and Ilya Vekhter (LSU); Senior investigators: John F. DiTusa, Juana Moreno, Sunggook Park, Jagannathan "Ram" Ramanujam, David P. Young, and Jiandi Zhang (LSU). Status: Pending. Submission date: 01/2011. Beginning date: 09/2011. Ending date: 08/2014. Amount requested: $4,149,100. Title of

award: MIRT: An Integrated Approach to the Discovery of Emergent Quantum Phenomena. Grantor: NSF.

- H. Fotso, M. Jarrell, J. Moreno, S. Pathak, V. Rousseau, D. E. Sheehy, K.-M. Tam and S. Yang (LSU); Z. Bai, C.-C. Chang, S. Chiesa, R. Scalettar and Andres Tomas (University of California, Davis); K. Tomko (Ohio Supercomputer Center); D. Galanakis (Nanyang Technological University, Singapore); and F. F. Assaad (Universitat Wuerzburg, Germany). Status: Pending. Submission date: 04/2011. Beginning date: 07/2011. Ending date: 06/2012. Amount requested: 16 million SUs. Title of award: Simulations of Strongly Correlated Systems. Grantor: NSF thought the TeraGrid.
- "Idea Place and Summer Science Institute and LA GEAR UP Partnership" proposal sent to NASA, $51,803.18. 04/01/11-08/31/11. PI: Glenn. Beer, Co-PIs: Lindsey Keith-Vincent, Neil Crews and Daniela Mainardi. Status: Awarded
- Shared Memory Computational Infrastructure for Computational Chemistry and Materials Science Education, BoR-Enhancement, $68,599. PI: Bala Ramachandran, Co-PIs: Pedro Derosa, Collin Wick, Daniela Mainardi. Status: Awarded
- "RET Site: NERO II: Nanoscience Education and Research Outreach II", **NSF**, $498,856, PI: D. Mills, Co-PIs: D. Mainardi and E. Murray. Submitted 02/2011. Status: Pending
- "Corrosion Mitigation in Concrete using Electrokinetic Nanoparticle Treatment", **NSF**, $601,698, PI: D. Mainardi, Co-PIs: H. Cardenas, J. Kanno. Submitted 02/2011. Status: Declined
- "Louisiana Tech's Research Scholar's Program: Creating Competencies, Curricula, and Careers Through University/K-12 Research Partnerships", **NSF**, $2,819,327, PI: D. Mills, Co-PIs: D. Mainardi. Submitted 07/2010. Status: Declined
- B. Ramachandran, Collin Wick, J. Palmer, D. E. Hall, and Y. Lvov: Removal of trace water from cooking oils, $50,000, Frymaster Corporation, January 1-June 30, 2011. Funded.
- Derosa: "Multiscale Modeling of Nanocomposites", AFRL, $100,000, 10/01/2010-12/31/11. Funded.
- Derosa: "JFAP Summer Research Program (2010)", NSF-BoR, $60,381, 05/01/10-09/30/10. Funded.
- Derosa: "Microscale Radiological, Environmental, and Biological Monitoring Microdevices for NASA Commercialization", BoR-NASA, $1,500,000. 08/01/2011-07/31/2014. Declined.
- Z. Dick Greenwood: DoE Award: $750,000/3 yr 07/01/10-06/30/13 for "Research in Experimental Particle Physics"
- Z. Dick Greenwood: DoE ARRA Award: $33,860 supplemental proposal for research infrastructure, awarded in July 2010.

Economic development
Industrial partnerships

Progress on the establishment of the NSF Center on Visual and Decision Informatics (CVDI), a planned Industry-University Cooperative Research Center

Establishing an IUCRC remains one of LI's salient economic development performance measures. The CVDI not only accomplishes that metric, but is also well aligned with the technical directions of the LI.

CVDI's mission is to research and develop next generation visual and decision support tools and techniques within large-scale data-centric environments to enable decision makers in government and industry to fundamentally improve the way their organization's information is interpreted and analyzed. CVDI will bring together, analytic, visual and perceptual techniques by advancing the state-of-the-art in the research fields of Information Visualization, Visual Analytics and Automated Analysis. Research conducted within CVDI will lead to the creation of a set of new Decision-Making Environments (DME)

that allow users to explore and customize large-scale information streams in a variety of modalities and to gain better insight to information.

Establishment of an NSF I/UCRC requires achieving several milestones. UL Lafayette received NSF approval of its Notice of Intent and was awarded a Planning Grant in 2008. Our academic partner, Drexel University, crossed those same milestones in 2009. Since then, both universities are actively recruiting potential industry partners, by organizing several pre-planning meetings and promoting the benefits to industry of the NSF I/UCRC model, both as a catalyst for innovation and economic development.

On May 3 - 4, 2011 UL Lafayette and Drexel conducted the I/UCRC Planning Meeting, with NSF and industry representatives in attendance. It was held at Drexel in Philadelphia and was attended by 9 potential center members from ULL side and 6 prospects from Drexel side. A number of research projects were presented for industry consideration and, through discussions at the meeting as well as exchange of additional information companies requested (after the meeting), we have arrived at a prioritized list of the research projects. With this, the NSF's requirements for successful completion of a Planning Meeting have been met. Industry partners have ranked projects proposed and led by Dr. Raju Gottumukkala (LI Computational Scientist) and Dr. Ramesh Kolluru (LI Co-PI) as among their highest priority projects. The LONI Institute is indeed stimulating the development of the CVDI. At UL Lafayette, Dr. Kolluru leading the efforts at recruiting industry as Site Director for the proposed center; Dr. Vijay Raghavan will serve as Director of the CVDI.

We are now at the stage of obtaining Letters of Commitment from the prospective members. Both Drexel and UL Lafayette must obtain a minimum of 5 letters (for a total of 10) of commitment for us to be eligible to submit the final NSF proposal. We believe that we will both exceed that requirement. It is our understanding that, since the Planning Meeting requirements are met, the approval of the Center is almost certain as long as both academic partners receive the required number of Letters of Commitment, which we expect will be accomplished by end of this month. We will, then, submit the full proposal by Sept. 26th; we expect the Center to kick-off in Spring 2012.

We excited to report that we are leveraging LI investments to facilitate the development of the CVDI, based on synergies between the goals of NSF-CVDI and the LONI Institute. Further information on NSF CVDI is also available at: http://nsf-cvdi.louisiana.edu.

The following companies have committed to be partners with the proposed Industry/University Collaborative Research Center for Visual and Decision Informatics.

- Sound Operating Systems
- AstraZeneca
- Elsevier
- Forward Link
- GE Healthcare
- Henry Safety Technologies
- Huawei
- IBM
- Johnson & Johnson
- Louisiana Department of Revenue
- Louisiana Immersive Technologies Enterprise
- National Board of Medical Examiners
- Stuller, Inc.
- FirstCall Technologies

Removal of trace water from cooking oils, Collin Wick and Ramu Ramachandran (LA Tech)
This was a partnership with Frymaster Corporation in Shreveport. The project involved computational modeling on LONI computers by Wick and Ramachandran, and experimental work by both researcher as well as other collaborators. The research was done under a Non-Disclosure Agreement and so the details cannot be provided in this report.

Other industrial partnerships
At SUBR:
- IBM
- Oracle

At ULL:
- James Lee Witt Associates
- GeoComp Corporation
- LA 1 Coalition, Inc.
- Maritime Institute for Emergency Monitoring and Response
- Fusion Technologies/Premiere Performance Systems

Industry contracts/grants
Removal of trace water from cooking oils, $50,000, Frymaster Corporation, January 1-June 30, 2011, LA Tech.

Collaborations
At Tulane:
- John Kessler (University of Arizona, Physics). Swimming organism experimentalist.
- Robert Dillon (Washington State University, Mathematics). Computational models of swimming organisms.
- Luis Cisneros (Univ. of Arizona, Physics). Postdoc with J. Kessler (above)
- Martin Bees (Univ. of Glasgow, Scotland, Mathematics). Numerical methods for biological flows.
- Ricardo Ortiz (Univ. of North Carolina, Mathematics). Numerical methods for biological flows.
- Priya Shilpa Boindala (Georgia Gwinnett College, Mathematics). Former student of mine.
- Bree Cummins (Tulane University, mathematics). Agent-based models for disease transmission.
- Hoa Nguyen (Tulane University, Mathematics). Numerical methods for biological flows.

From Francisco Hung, LSU:
- F. Ehrenhauser, M. J. Wornat, K. T. Valsaraj, L. Thibodeaux, K. Nandakumar (Chemical Engineering, LSU)
- M. Warner, S. Das, J. Y. Chan, J. C. Garno, P. S. Russo, E. Nesterov, D. Zhang, Z. Wilson, G. Stanley (Chemistry, LSU)
- W. Plummer, R. Jin, J. DiTusa, I. Vekhter, D. Young, J. Zhang, (Physics, LSU)
- T. Monroe (Biological and Agricultural Engineering, LSU)
- K. G. Kousoulas (School of Veterinary Medicine, LSU)
- J. E. Bara, C. H. Turner (Chemical and Biological Engineering, University of Alabama)
- M. Jeffries-El (Iowa State)
- K. Johnston, S. Bryant, R. Bonnecaze, T. Truskett, Q. Nguyen (UT Austin)
- S. Garoff, L. Walker, S. Anna (Carnegie Mellon)
- L. Pratt, K. Papadopoulos, V. John, H. Ashbaugh, N. Pesika (Tulane)
- J. Lee, G. John (CUNY)
- G. Bothun, A. Bose (U. Rhode Island)
- P. Somasundaran (Columbia)

- B. Tansel (Florida Intl. Univ.)
- S. Raghavan (Maryland)
- R. Weiss (Georgetown)
- P. Kilpatrick (Notre Dame)
- M. Tsianou, P. Alexandrides (Univ. Buffalo)
- K. Linden (U. Colorado)
- C. Hall (NC State)
- B. Prud'homme, P. DeBenedetti (Princeton)
- McCormick (Minnesota)
- L. Dai (ASU)
- T. Dinsmore (U. Mass Amherst)
- R. Hurt, A. Kane (Brown)
- R. Larson (Michigan)
- A. Roy (CAMD-LSU)
- N. Alcantar, R. Toomey (U. South Florida)
- C. McCormick (Univ. Southern Miss.)
- R. Krishnamoorti (Univ. Houston)
- C. Roberts, R. Gupta (Auburn)
- J. Chen (State Key Laboratory of Water Environment Simulation, School of Environment, Beijing Normal University, China)

At LA Tech:

- Lawrence Pratt, Fisk University, Nashville, TN, (collaborates with Ramachandran)
- Professor Adrain Bejan, Duke University (collaborates with Dai)
- Professor Da Yu Tzou, University of Missouri (collaborates with Dai)
- Assistant Professor Le Zhang, Michigan Tech University (collaborates with Dai)
- Daniela Mainardi has established collaborations in the areas of **Energy Conversion and Storage** with Prof. Suddhasatwa Basu, IIT Delhi India. At this time they are working together to decipher reaction mechanism in direct alcohol fuel cell (DAFC). IITD and LATech would start collaboration through short visit of Ph.D. students from both sides by taking help of funding available in individual countries and as well as sponsored projects already funded. The data generated from IIT Delhi on DAFC will be shared with LATech to model reaction mechanisms and electrochemical characterization results (cyclic voltammetry, impedance spectroscopy etc.) using quantum chemistry and a kinetic Monte Carlo approach.
- Rajiv Berry, AFRL (collaborates with Derosa)
- Hua-Jun Fan, Prairie View A&M University (collaborates with Derosa)
- Tahir Cagin, Texas A&M (co-editor of a book with Derosa)
- Horst Severini and Pat Skubic from the Univ. of Oklahoma (collaborates with Greenwood)
- Joel Snow from Langston University, OK (collaborates with Greenwood).

At ULL:

- Dr. Vijay Raghavan, Distinguished Professor, Center for Advanced Computer Studies, University of Louisiana at Lafayette. The LONI Computational Scientist and the lead PI at UL Lafayette work very closely with Dr. Raghavan in establishing an NSF I/UCRC Center for Visual and Decision Informatics at the University of Louisiana at Lafayette in partnership with Drexel University.
- Dr. Ryan Benton, Research Scientist, Center for Advanced Computer Studies, University of Louisiana at Lafayette, joint LONI Institute project with the LONI Computational Scientist
- Dr. Baker Kearfott, Professor, Department of Mathematics and Statistics, University of Louisiana at Lafayette, Joint LONI Institute project with the LONI Computational Scientist

At SUBR:

- Dr. Shengmin Guo: LSU ME on TBC and MAX phase simulations;
- Dr. Kun Lian: CAMD LSU on carbon coated Cu catalyst simulation;
- Dr. Uppu: SU Environmental Toxicology on apocynin and BPA docking and MD simulations.

At LSU, S. Jha:

- National: Dan Katz, Jon Weissman, Manish Parashar, Yogesh Simmhan
- International: Omer Rana, Peter Coveney, Dieter Kranzmuller, Marc Santcroos, Simon Dobson, Jon Blower
- Louisiana: Tom Bishop, Rajib Mukherji, Hideki Fujioka

C) Opportunities for faculty recruitment, retention and development, as well as post-doc, graduate and undergraduate student training

One of Louisiana Tech's LI hires, Dr. Abdelkader Baggag, resigned in October 2010. A search was initiated to fill this position with a computational scientist who will advance one or more of the scientific themes of the LONI Institute. As of April 2011, we were successful in recruiting Dr. Thomas Bishop, a computational biology researcher with degrees in Physics, Mathematics, and Chemistry, as Associate Professor of Chemistry and Physics. Dr. Bishop will begin his career at Louisiana Tech on July 1, 2011.

Dr. Collin Wick is also a LI Faculty at LA Tech.

LSU will be hiring Dr. Michal Brylinski, he will start on January 2012. Dr. Brylinski obtained his Ph.D. in Chemistry from Jagiellonian University, in Krakow, Poland, in 2006. His research interests include systems biology, chemical systems biology and chemoinformatics; drug discovery and design; ligand docking/screening; ligand comparative modeling; protein function inference; protein structure prediction; protein evolution; and high performance computing.

ULL is still looking for a suitable candidate to fill in the LONI faculty position in the Engineering department.

Students doing internships

Tulane:

- Amanda Foy (June 2011). Undergraduate student working with R. Cortez
- Christina Yee (June 2011). B.S. May 2011. Internship at Areté Associates (science and engineering company)
- Brooks Fowler (June 2011). B.S./M.S. 2011. Position at Brainlab.

LA Tech:

- Ram Dhullipudi, LI graduate fellow – LHC at CERN, Geneva
- Rajiv Subramaniam, LI graduate fellow - LHC at CERN, Geneva
- Anirvan Sircar - LHC at CERN, Geneva
- Sudapa Laosooksathit – University of Hertfordshire, UK
- Fred Moxley, NASA, Washington, DC
- Muhammad Assad, LSU Health Sciences Center, Shreveport
- Joshua Brown, Summer 2010 and Summer 2011
- David Cossey, Summer 2011

SUBR:

- Kimberlee Lyles
- Vani Panguluri

UNO currently has three CS students (undergraduates) working as interns in local IT companies. None of those three students was working with an LI associated faculty member, however. We are currently filling two internships with Eurofins which will be in microbiology or analytical chemistry. It is possible that a student working with one of the LI associated faculty members may fill that internship.

Visit to national labs

- Box Leangsuksun made multiple visits to Oak Ridge National Labs to collaborate on projects funded by the National Science Foundation.
- Collin Wick spent one month at Pacific Northwest National Labs during Summer 2010.
- Pedro Derosa visited Wright Patterson Air Force Base in Dayton, OH as part of his collaboration on a multi-university grant funded by the US Air Force.
- Dr. Yang and his student Jialin Lei visited LBNL Berkeley Lab in May 2011 performing HP experiments at beamline 12.2.2 on Cr-Y alloy.
- Dr. Yang and Dr. Guo were invited to visit and make a talk each at NETL Albany Lab in June 2011.

Scientific Computing Course

Allen, Jha co-taught a new graduate course in scientific computing that was taught during Fall 2010 at Louisiana State University. (Other instructors from LSU included Benger, Hutanu & Schnetter) The course was designed to provide students with a broad and practical introduction to scientific computing which would provide them with the basic skills and experience to very quickly get involved in research projects involving modern cyberinfrastructure and complex real world scientific problems. The course, which was taken by thirteen graduate students, covered basic skills, networks and data, simulations and application frameworks, scientific visualization, and distributed scientific computing. Notable features of the course include a modularized team-teaching approach, and the integration of national cyberinfrastucture with teaching.

HD video courses:

One course was offered during Fall 2010:

Computational Solid State Physics by Rongying Jin (LSU) and Cyrill Slezak (Hillsdale College, Michigan).This a graduate survey course covering subjects ranging from point group theory, scattering, and Fermi liquids, to lattice and spin dynamics. Numerical simulations are used throughout the lectures and homework problems. A total of 14 students at LSU (12) and Hillsdale College (2) were enrolled in the course.

Three courses were offered during Spring 2011:

Advanced Solid State Physics with Computation by Mark Jarrell (LSU). Website: http://www.phys.lsu.edu/~jarrell/COURSES/ADV_SOLID_HTML/course_advss.html. This course covers the core ideas which define many-body theory for condensed matter, including Green functions, bosonization, Feynman Dyson perturbation theory, coherent states and path integrals. Non-equilibrium transport theory was also covered due to its importance in several LA-SiGMA and LONI Institute projects. Related numerical methods are discussed and used throughout the course. One student from Louisiana Tech and two from Tulane University participated through synchronous video. About ten from LSU also attended the course.

Computational Physics: Computing for Petascale Systems by Karen Tomko (Ohio Supercomputer Center) and Juana Moreno (LSU). This course covers high performance computing (HPC) and the techniques used in designing and implementing computationally intensive applications on HPC systems.

High performance systems including traditional parallel supercomputers, multicore-based Linux clusters, and hardware accelerators (such as GPUs and FPGAs) are discussed. The course focuses on parallelization and memory access optimization for computationally intensive applications in science and engineering. Thirteen students from LSU participated in this course.
As the final project for this course 5 of the students began to develop Accelerated Physics and Chemistry Codes Using Graphic Processing Units (GPU) and CUDA. CUDA has already been used to accelerate non-graphical applications in many science domains with prototype speedups of 30. We hope to achieve heterogeneity with the addition of CUDA code to the current implementation of our codes.

Simulations of Quantum Many-Body Systems III by Matthias Troyer (ETH Zurich) and faculty at the Ludwig-Maximilians-Universitat, Munich; Ecole Normale Superieure, Paris; Max Planck Institute for the Physics of Complex systems, Dresden; University of Massachusetts, Amherst; University of Wyoming; and Louisiana State University.
Website: http://wiki.phys.ethz.ch/quantumsimulations/notesspring2011. This course is an introduction to simulation methods for quantum many-body systems in condensed matter physics, taught by experts of the various methods. This class is the third semester of a three-semester course shared by tele-teaching among seven institutions. This spring the course had over 40 students from LSU, Tulane and LA Tech. In particular this spring the course covered: equilibrium Green Functions methods and the Dynamical Mean Field Approximation, taught by Mark Jarrell (LSU); Diagrammatic Monte Carlo by Boris Svistunov (University of Massachusetts, Amherst); Continuous Time Quantum Monte Carlo by Philipp Werner (ETH); and Density Functional Theory for materials science, by Thomas Schulthess (ETH).

LI/LA-SiGMA Seminar Series
The LONI Institute/LA-SiGMA seminar series started in September 2010 and is designed to provide a strong platform for interactions between various elements of the LONI Institute and LA-SiGMA . It is also expected to improve the general research atmosphere, and provide Louisiana researchers a greater exposure to cutting edge methodologies. The seminars are being conducted on a revolving basis where the participating sites take their turn in hosting a speaker. Out of state speakers are also welcome as they can contribute strongly to broader goals of the LONI Institute and LA-SiGMA. The talks were coordinated by Dr. Bhupender Thakur during Fall 2010, and by Dr. Dentcho Genov during Spring and Summer 2011. The talks are broadcast over the Access Grid and are open to all sites. The talks are meant to bring a greater degree of cohesion and a better collaborative atmosphere. LA-SiGMA is also facilitating an upgrade of HD devices so that in future, these talks can be better disseminated.

Tutorials
Shantenu Jha delivered the following tutorials:

- "Introduction to SAGA on EGI", EGI Workshop, Vilnius, April 2011
- "SAGA Tutorial", Joint TeraGrid and LONI Tutorial/workshop

Workshops

Beowulf Boot Camp
The LSU Center for Computation & Technology (CCT) , supported by the LONI Institute, hosted the fourth **Beowulf Boot Camp** June 6-10 on the LSU campus. This exciting summer education opportunity offers high school teachers and students a unique opportunity to work with advanced research technology not usually available in a typical classroom setting.

During Beowulf Boot Camp 2011, students worked hands-on with LSU Department of Computer Science Professor Thomas Sterling, a former NASA scientist who invented the Beowulf supercomputing cluster, and Dr. Steven Brandt, a computational scientist in the CCT who specializes in programming, as well as

other researchers from the CCT. The students learned how to use supercomputers for research, develop and run basic applications and experiment with computer science techniques.

Students engaged in the following activities:

- building a computer cluster from scratch
- installing the Linux operating system on the computer they've built
- connecting computers put together by their peers to make a Mini-Supercomputer
- learning how to program a Mini-Supercomputer
- interactive activities to help understand how Parallel computing works in Supercomputing
- running performance benchmarks to determine how your cluster ranks in comparison with the Fastest and Largest supercomputers in the world
- programming in Python.

There were 39 participants total (2 high school teachers; 37 students). Twenty people were from outside Baton Rouge, and surrounding areas (Slidell, Covington, Madisonville, New Orleans, New Iberia, Broussard, Maurice, Gueydan, Vacherie, Charenton), 19 from Baton Rouge and surrounding areas. There were 3 Females; 36 Males, with one underrepresented minority (African American).

Workshop on Density Functional Theory
Faculty from LSU, LA Tech, and Tulane are hosting the "LONI Institute Workshop on Density Functional Theory", July 23rd to 27th, 2011 on the campus of Louisiana State University. The conference is sponsored by the LONI Institute (LI).

It will be a pedagogical workshop designed to expose graduate students and postdocs to several flavors of electronic structure calculations in a holistic way. In particular, it will be accessible to graduate students and postdocs in condensed matter physics, chemistry and materials engineering, who may not have prior knowledge of Density Functional Theory (DFT) methods. We are targeting no more than 35-40 students/postdocs from all LI and LA-SiGMA institutions.

Five experts in DFT methods, John Perdew, Tanusri Saha-Dasgupta, Shobhana Narasimhan, Mel Levy, and Weitao Yang, will present two two-hour-long pedagogical and expository lectures, and complement their lectures with hands-on sessions in which participants will learn to perform simple calculations. We will have lecture and hands-on computational labs for around 7 or 8 hours each day, and the format will allow plenty of time for discussions.

Virtual School of Computational Science and Engineering (VSCSE)
The LONI Institute is also involved in the VSCSE workshop and will be covering the registration of some students.

The VSCSE provides courses and learning resources to help computational science students, post-docs and young professionals from all disciplines use emerging petascale computing resources to address real domain science problems.

The summer courses for 2011 are:

- Petascale Programming Environments and Tools (July 12-15)
  including two online short courses, Introduction to MPI and Introduction to OpenMP
- Proven Algorithmic Techniques for Many-core Processors (August 15-19)
  including a short online course, Introduction to CUDA

These courses will be delivered to a number of sites nationwide (including LSU) using high definition video conferencing technologies, allowing students to travel to a number of convenient locations where they will be able to work with a cohort of fellow computational scientists, have access to local teaching assistants and interact virtually with course instructors. Please visit http://www.vscse.org/summerschool/2011/index.html for more information.

Indo-US partnership in computational materials science
LONI Institute faculty from LSU, LA Tech, and Tulane, in collaboration with Professors Vidhyadhiraja Sudhindra from JNCASR, Bangalore, and Tanusri Dasgupta from SNBose Centre, are putting together a request for funding from the Indo-US Science and Technology forum (IUSSTF) to form an international virtual graduate research and education centre focused on computational materials science. The IUSSTF provides two-year grants to seed such centers. Center funds will be used to support long and short term visits of US faculty to India and vice versa, as well as student exchanges. Participants in the project will share students, courses and group meetings via synchronous and asynchronous video, and codes via SVN repository. In addition to the LONI Institute the other US partner is the Louisiana Alliance for Simulation Guided Materials Applications (LA-SiGMA). Near the end of the seed grant, longer term support for the Centre will be requested from the NSF/Gov't of India Department of Science & Technology (DST) Joint Program.

LONI Training
LONI tutorials and workshops are taught and coordinated by HPC@LSU staff at LSU, and supported by the LI CSs at the different universities. During the past year, the following tutorials were given:

Fall 2010
- Introduction to HPC: Account Allocation and Management
- Job Management with PBS/LoadLeveler
- Introduction to MPI
- Advanced MPI
- Introduction to Cactus
- Introduction to Gaussian
- Introduction to OpenMP
- Advanced OpenMP
- Introduction to Globus
- Introduction to HPC Visualization: tools, resources
- Introduction to SAGA

Spring 2011
- Introduction to HPC: Account Allocation and Management
- Job Management with PBS/LoadLeveler
- Introduction to MPI
- MPI Part 2
- Molecular Dynamics: Programming to Production
- Introduction to Hybrid Programming
- Introduction to CPMD

Summer 2011
- Introduction to HPC
- Introduction to HPC user environment
- Introduction to Parallel Programming

- Introduction to OpenMP
- Molecular Dynamics
- Electronic Structure Calculations

The workshops were:

Spring 2011
- February 17 & 18 at Southern University, Baton Rouge. 27 people joined the training in SU.
- March 24 & 25 at Tulane University, New Orleans.

D) Partnership activities

LA-SiGMA
The current NSF EPSCoR RII grant was funded in October 2010. This grant, the Louisiana Alliance for Simulation-Guided Materials Applications, LA-SiGMA, is a spinoff of the LONI Institute, and complements it by adding support for the research groups of the faculty hired by the LI grant.

The Alliance members are LSU (lead institution), Grambling State University (GSU), LA Tech, UNO, SUBR, Tulane, and Xavier University (Xavier). GSU, SUBR, and Xavier are classified as "historically black colleges and universities" (HBCU) and have large underrepresented minority enrollments.

LA-SiGMA creates a statewide research and education program focusing on (1) electronic materials, (2) energy materials, and (3) biomolecular materials. Within the overall theme of "computational materials science," these science drivers emerged as clear areas of strength through a statewide solicitation that yielded over forty multi-institutional whitepapers from teams of researchers. The majority of these teams included computational and experimental researchers, providing a strong foundation for the proposed research program that relies on close collaboration between theorists, computational scientists, and experimentalists. The Alliance capitalizes on the jurisdiction's Cyberinfrastructure (CI) and past investments in experimental and computational materials science. Program objectives include: building the next generation of experimentally validated formalisms, algorithms, and codes for multiscale materials simulations; implementing them on present and next generation supercomputers; and educating the next generation of a highly skilled workforce of materials scientists and engineers.

Website: http://lasigma.loni.org

IV. CONTRIBUTIONS

Summarize efforts made to
a) build research and education capacity,
b) secure external federal and private-sector funding,
c) build infrastructure,
d) contribute to economic development, and
e) ensure project sustainability over the long term.

In summary, in its fourth year, the LONI Institute has made great strides.

The LONI Institute is part of a coordinated effort to *build research and education capacity* in computational sciences research and education throughout the state of Louisiana. The three pillars of this project are the LONI network, the LONI Institute and the recent NSF LA-SiGMA award. The LONI

network provides the high-speed connections required to connect this statewide virtual graduate research and education project. It also provides the computational resources. The LONI Institute provides the resources to hire the requisite computational sciences faculty and staff. The LA-SiGMA award recently secured by LONI Institute faculty is the third pillar. It provides funding which supports LONI Institute researchers and their research groups. LONI Institute and LA-SiGMA allow these researchers to leverage the LONI hardware in their research and to train the next generation of computational scientists for Louisiana.

LONI Institute has been very successful in its efforts to *secure external federal and private sector funding*. The LA-SiGMA award is the most successful such effort with $20M over a five year term. With this award, the total federal funding raised by LONI Institute members now exceeds $35M.

The LONI Institute is an essential part of the state's effort to build its research *infrastructure* in the computational sciences. It has successfully recruited new research faculty into the state, and has contributed to the education of students. It is building sustained new collaborations between these researchers and attracting new funding sources to the state.

Through these efforts the LONI Institute is contributing intellectual capital that spurs *economic development*. LONI Institute members at ULL are in the final stages in the development and approval of an NSF Center on Visual and Decision Informatics (CVDI), a planned Industry-University Cooperative Research Center. These efforts are enhanced by the LONI Institute training workshops, numerous courses made available to students and researchers throughout the state via synchronous video (distance learning), and a regular bi-weekly seminar series.

The impact of the LONI Institute is significant. During very difficult economic times, it has allowed Louisiana Institutions to hire leading researchers in the computational sciences. These researchers have attracted a significant amount of funding which is being used to train a new generation of computational sciences researchers who will *sustain* the Institute into the future.

V. PROJECT REVISION

Provide a listing of and explanation for any significant changes in the work plan for upcoming year, including any changes in the amount of investigators' time devoted to the project. If you made significant changes to the project design as outline in the proposal during the past year, please list and explain the changes, the purposes for the changes, and the results.