Third Annual Report
LONI Institute PKSFI Project
July 1, 2009 – June 30, 2010

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 Ramachandran, Neven Simicevic
Southern University at Baton Rouge	Michael Stubblefield, Ebrahim Khosravi, Habib Mohamadian
Tulane University	Gary McPherson, Ricardo Cortez, Lisa Fauci, Donald Gaver
University of Louisiana at Lafayette	Ramesh Kolluru, Devesh Misra, Joe Neigel
University of New Orleans	Scott Whittenburg, Vassil Roussev, Stephen Winters-Hilt

Website: http://institute.loni.org

Introduction

In the third year of the LONI Institute (LI) the effort was concentrated at the research and education part of the project, as well as consolidating external funding as part of the sustainability of the project.

A major success of the project during the third year is the new NSF-EPSCoR RII award, an effort of the LI and Xavier University, that will start in the next few months. This award, "Louisiana Alliance for Simulation-Guided Materials Applications (La-SiGMA): Leveraging Next Generation Supercomputing to Study Complex Emergent Phenomena in Novel Materials" is the largest award ever received in the State of Louisiana, for a total of $20M for five years shared by researchers at all of the LI sites.

Other successes include the addition of Xavier University as an LI member. Xavier University is the only NSF Center of Excellence in the state, and the most successful HBCU in the nation. According to the U.S. Department of Education, Xavier continues to rank first nationally in the number of African American students earning undergraduate degrees in both the biological/life sciences and the physical sciences.

Most of the LI faculty, staff, and students for the project were recruited during the first year of the LI. The majority of the faculty started during the second year of the project (fall 2008), and the University of Louisiana at Lafayette (ULL) hired an LI Faculty member during the third year of the LI. Unfortunately, not all the faculty positions have been filled. One position at Louisiana State University (LSU), and one position at ULL remain open. Hiring freezes and the current budget situations in the State of Louisiana have hindered our efforts. We, however, have successfully filled all the (six) LI Computational Scientist (CS) positions at all the LI sites members. We have offered LI Graduate Fellowships every year, and Senior Investigators (SIs), and LI Faculty coordinate the search and, starting in the third year of the project, as stated in the project proposal, they have chosen two students per LI site (one from the LI grant, and one from matching funds at each institution). Even though the goal is to have a total of twelve students during the third year, the search at ULL was unsuccessful, similarly to the one at Southern University at Baton Rouge (SUBR) and we had a total of 9 students.

We continued our second year of LI projects, where the LI CS work with different researchers across the state for a period of one year on projects that were selected by the LI scientific committee and the LI CSs themselves. We have also introduced an assessment system for the Graduate Fellowships and LI Projects, and we will kick-off our LI/La-SiGMA Seminar Series on the Fall. This seminar series will happen at the different LI sites, and will be broadcasted to all LI sites via the Access Grid.

Outline of this report

The Board of Regents has requested reports that provide information in the following sections: (1) Personnel; (2) Activities and Findings; (3) Contributions; and (4) Project Revision. The LI project has many milestones and deliverables that do not necessarily match such a format. Therefore, in the following sections, we discuss in detail the progress towards these specific milestones and deliverables, and we have attempted to group in roughly this order. However, we have combined sections (1) and (2), and reported on the requested activities as appropriate.

Progress on LONI Institute Specific Milestones and Deliverables

As stated in the proposal for this project, the LI has defined numerous metrics to measure project progress and success. These metrics include the hiring of faculty and researchers, creating statewide interdisciplinary research projects and obtaining federal follow-on funding for such, developing corporate partnership programs and start-up companies, developing and following interdisciplinary and multi-institutional collaborations, and creating new educational programs. The performance measures are discussed in detail below, accompanied by project milestone estimates.

At the end of each item, we provide information collected for this third annual report. We highlight specific progress by institution where notable.
This report mostly contains work done by LI faculty, staff and students, but also data from people who are associated with the LI.

1. PERSONNEL, ACTIVITIES AND FINDINGS

In this section, we have combined the first two required sections of the report: 1. Personnel, and 2. Activities and Findings. We provide a description of all the personnel hired during the year, along with activities and findings, as appropriate.

1.I. Personnel Objectives, Metrics and Success Criteria

According to our strategic plan, we have the following personnel Objectives, Metrics, and Success Criteria for measuring when these objectives are achieved, as well as dates expected:

Objective	**Metric**	**Success Criteria**	**Status**
LONI Fellows	Full-time faculty hires, 2 per institution	6 by EOY2; 12 (total) by EO Y3. Nucleation of 6 new multi-institutional research groups by Y3.	10 fellows hired by the EOY3 (Sec. 1.I.a).
Development Coordinator	Individual hired	1 hire, Fall Y1; new hire in 6 months if position becomes vacant	Individual was hired in Y1.
LI Graduate assistantships	Graduate students funded by Institute	6 in each 2 year period; 18 students total over	21 Graduate Fellow positions funded so

		life of project	far (Sec. 1.I.c).
LI Computational Scientist	Individual hired	6 hired in Fall Y1; new hire in 6 months if position becomes vacant	6 CSs hired at EOY3 (Sec. 1.I.d).
LI-seeded growth of LONI to national status	Receive federal funding for additional staff	12 staff funded from federal sources by EOY5	12 positions funded in Y2 (Sec. 1.I.b).

1.I.a) Full-time faculty hires

During Y1, five LONI Fellows (LI Faculty) were hired, with most of them having a start date in Y2. These LI Faculty were introduced in the first annual report, and are Drs. Abdelkader Baggag, Dentcho Genov, Mark Jarrell, Damir Khismatullin, and David Mobley. During Y2, four more faculty were hired, with two having a start date in Y3, and are Drs. Caroline Taylor, Christopher Taylor, Zhenyu Ouyang, and Rachel Vincent-Finley.

During Y3, ULL hired *Dr. Scott Duke-Sylvester*, for the Department of Biology in the college of Science. Dr. Duke-Sylvester received his MS in Mathematics and his PhD in Ecology and Evolutionary Biology and the University of Tennessee at Knoxville. While there, he worked on computational models of plant population dynamics in wetland ecosystems. The study system for this research was the Florida Everglades, for which he produced spatially explicit landscape scale models used to evaluate the effect of alternative Everglades restoration plans. He did his post-doctoral work at Emory University. While there, he branched out into studying the dynamics of infectious diseases (ID). In particular, he examined the spatial dynamics of raccoon rabies produced by cyclic patterns of increasing and declining density of the raccoon population associated with seasonal breeding. At the University of Louisiana at Lafayette, he is currently moving into the evolution of infectious diseases. RNA viruses, such as rabies and west nile virus, experience rapid rates of molecular substitution that occur on a time scale that is compatible with the ecological dynamics of disease spread. Scott is interested in how the evolutionary dynamics of a pathogen are influenced by the contemporaneous process of infection and disease spread.

In addition, the committee at ULL has interviewed multiple candidates for the LONI faculty position within the College of Engineering. The finalists for both positions have been identified and job offers are being made for a starting date of Fall 2010.

Collin Wick, an Assistant Professor in Chemistry, at Louisiana Tech University (LA Tech), received an offer from PNNL. Because of the severe budget cuts to higher education this year, and because one of the most important goals of LI is to attract and retain intellectual capital in the computational sciences, a portion of the LI budget was used to make a counteroffer to Dr. Wick to retain him. The retention effort was successful and Dr. Wick is now counted as an LI faculty member.

LSU continue their search for a senior Computational Biologist. We received several excellent applications, and narrowed the field down to a short-list of four candidates. Unfortunately, the search had to be canceled again by the College due to budget cuts. This search remains a very high priority for the LI and the College of Sciences, and it will be renewed as soon as possible.

A description of the research done by LI Faculty can be found in appendix A.

1.I.b) Federal funding for additional staff

We have 12 staff positions currently funded by the LONI HPCOPS project from NSF. We refer you to http://www.hpc.lsu.edu/about/staff . With the new NSF-EPSCoR RII grant, five additional federally-funded staff will be supported in addition to hiring a very large number of students, postdocs and faculty..

Sumeet Dua, LI SI, is funding a postdoc (Pradeep Chowriappa) through NIH/INBRE: INBRE-Data Mining Microarray Gene Expression Data For Physiological Discovery ($770,770), INBRE - administrative support ($304,003)

1.I.c) LI Graduate Fellows

The LI supports LONI Institute Graduate Student Research Assistants. Assistantships are available at all member institutions. Research can be in any area of science, engineering, social sciences, or arts and humanities, although the fellow awards are intended to support graduate students whose research projects require access to high-end computing facilities, networks, distributed data archives, and more generally cyberinfrastructure. The awards include a $20,000 stipend and tuition waiver.

The LI Graduate Student Fellows were selected on the basis of
- Excellence in research in the disciplines
- Potential to utilize and advance the infrastructure under development across LONI
- Promise for external funding in the future
- Potential to meet the metrics for success of the LI

As explained before, the search for graduate fellows was unsuccessful at ULL for both positions, and at SUBR for one position. There were only two students applying for the ULL fellowship, and, according the LI scientific committee, none of the candidates had a strong application in order to obtain the fellowship. The committee agreed that we should put out another call for the LI Fellowship at ULL to try to obtain more applicants, which again, was unsuccessful. The situation was similar at SUBR.

Below, we show a list of the Y3 LI Graduate Student Fellows.

Graduate Fellow	**Institution**	**Field**
Steven Baker	LA Tech	College of Engineering and Science
Wei Huang	LSU	Biological Science Department
Salman Javaid	UNO	Department of Computer Science
Pavel Klimovich	UNO	Department of Chemistry
Hongzhi Lan	Tulane	Department of Biomedical Engineering
Kimberlee Lyles	SUBR	Department of Computer Science

Narate Taerat	LA Tech	Department of Computer Science
Shuxiang Yang	LSU	Department of Physics & Astronomy
Linghang Ying	Tulane	Department of Physics

We also provide a description of their research in appendix D.

For next year, we have set up a scoring criteria for the fellowship applications that would be specific enough to allow objective evaluations and yet broad enough to accommodate the diversity among the disciplines:

A. Research quality:
1. Alignment of proposed research with major open questions in the discipline.
2. Development of new formalisms, algorithms, and/or codes that would benefit the discipline.
3. Quality of the research description (a description aimed at a scientifically trained non-expert; must include a description of the computational challenges involved in the work and the cyberinfrastructure needed to make progress, such as massively parallel, large memory/disk, heterogeneous, leadership class, ...).

B. Academic standing and productivity:
1. Doctoral student? (We should fund MS students only at SUBR in disciplines where doctoral programs are not available)
2. Passed qualifiers?
3. Productivity of the applicant - papers, presentations (this weights the score in favor of senior PhD students in productive research groups)

C. Computing usage and needs:
1. Current and potential use of LONI infrastructure (does the applicant have a LONI account? Does (s)he have an allocation or is (s)he a member of an allocation? What is the approximate number of SU's consumed by the applicant in the preceding 12 months?
2. Does the applicant have accounts on any other supercomputers (NCSA, TACC, Pittsburgh SC, Minnesota SC, etc.)? What is the approximate number of SU's consumed by the applicant in the preceding 12 months?
3. Will the proposed research benefit significantly from the LONI infrastructure? How? (This could be addressed in the research description.)

D. Potential Impact of proposed research on LONI and the LONI Institute:
1. Will the products (software, papers, proposals) resulting from the applicant's work contribute to the advancement of the LI agenda?

1.I.d) LI Computational Scientists:

A crucial component of the LI is a strong contingent of advanced staff computational scientists. The LI proposal states that “the LI will support 6 PhD level computational scientists, typically with preexisting postdoctoral experience, to help State research groups take advantage of advanced cyberinfrastructure deployed across LONI and the nation. Distributed across the 6

participating campuses, these staff will be experts in the use of LONI hardware and cyberinfrastructure, including parallel computing, networks, visualization, grids, computational mathematics, and data management. These staff will work closely together, using HD video on all campuses, and will meet biweekly at LSU (supervised by SI Jha). Each of the computational scientists will be assigned 4-5 projects, with duration of 1-2 years each, so that significant progress can be made. These projects will be based on applications from all State campuses, with the applicants being encouraged to commit some internal resources. At least 50% of the projects will be in computational biology and materials science applications; however, we expect projects from other areas of importance to the State, in disciplines ranging from astrophysics, CFD, coastal science, medicine, engineering, digital arts and humanities, and business. This is a total of 70-90 projects over 5 years. Application teams from all State campuses and all companies will be eligible to apply for *LI* partnerships to develop applications that make use of LONI hardware and the staff."

In Y1, we hired 4 computational scientists, Dr. Hideki Fujioka (Tulane), Dr. Raju Gottumukkala (ULL), Dr. Shizhong Yang (SUBR), and Dr. Zhiyu Zhao (UNO). In Y2, LA Tech appointed Mr. Abdul Khaliq as the CS, who provides considerable amount of support for the modeling and simulation work in microstructures and devices, quantum chemistry, computational fluid dynamics, and electromagnetics. At LSU, the search continued during Y3, In the meantime, Dr. Shantenu Jha, Director for the Cyberinfrasctructure Development group at the Center for Computation & Technology (CCT) at LSU, appointed Dr. Tae-Woo Lee, as part-time CS for the LI. In June, the search concluded with the successful hire of Dr. Bhupender Thakur. Dr. Thakur obtained his Ph.D. from the University of Delaware in theoretical and computational nuclear physics. Dr. Thakur's research interests are nuclear structure theory and quantum many-body systems, numerical linear algebra and scientific computing, quantum computing, quantum information theory and statistical mechanics, parallel programming paradigms: MPI, OpenMP and other scalable implementations.

A description of the LI CSs research can be found in appendix B.

1.II. Research Objectives, Metrics and Success Criteria

Objective	**Metric**	**Success Criteria**	**Status**
LONI Computational Scientists	LI projects underway	12 new projects underway by EOY1; 18 new projects per year thereafter; at least 80 total; 25% projects permitted to be continued for new advances; 25% corporate	10 LI projects, and 14 starting at the EOY3 (Sec. 1.II.a).
State faculty, staff, and student trained and using LONI infrastructure	Number of applications for time, projects using compute, data, network, and software services	All LI projects use LONI, 12 personnel trained each year from each LI member, medical centers and community college system, 400 active LONI users from State by Y5	1031 users, 185 of them have logged on in the past 6 months (Sec. 1.II.b).

National proposals	LI-funded faculty-led national funding agency proposals, submitted and funded	50% of LI projects lead to proposals to agencies outside State (e.g., NSF, DOE, NIH) or industrial funding in Y2 and subsequent years; 2 proposals submitted per year, per LI Fellow, starting in Y2, 96 total, 10 new LI Fellows projects funded total	14 National awards for a total of $31M (Y1-Y3). CSs have 7 awards ($6M). See Sec. 1.II.c
Research computing project resources	Successful computational infrastructure/cycle applications	50% of projects lead to nationally-judged computational infrastructure awards in Y2 and subsequent years	See Sec. 1.II.c
Research publicity	Invited presentations and lectures outside LA	Each project leads to 2 presentations/lectures per year starting in Y2; 160 total	12 invited presentations. See Sec. 1.II.e
Scientific & Engineering Results	Peer-reviewed conference and journal publications that acknowledge LI support	3 per LONI Fellow per year; 1 per LI project per year; over 150 total	Numerous acknowledging LONI and LI (Sec. 1.II.d).
National Computing Center	LI personnel successful in obtaining federal funding	1 national federally-funded center, funded with at least $70M	None yet.
LI research impact	New non-LI-funded faculty working with LI	6 per year starting in Y2	See Sec. 1.II.f

1.II.a) LI Projects

During Y2, the LI put out a call for what we call LI projects http://institute.loni.org/liprojects.php), and by February 2008, the LI scientific committee had chosen 8 out of 23 projects for the LI Computational Scientist (CS) to work on. The criteria the committee used were the relevance of the research proposed, how the project would help the LI achieve its milestones, and an interdisciplinary, inter-, and/or intra-institutional component in each project, among others. We also asked for some of these projects to be adapted so that they will have one of these components, and these turned into other accepted projects. These projects continued until February 2009 (Y3), and the description was shown in the previous annual report:

1. "Infrastructure for Accurate and Efficient Binding Affinity Calculations"; PIs: David Mobley (UNO), Steve Rick (UNO), and Shantenu Jha (LSU); LI CS: Hideki Fujioka (Tulane).

2. "Spatial Modeling of the Dynamics of Invasive Nutria"; PI: Azmy Ackleh (ULL); LI CS: Raju Gottumukkala (ULL).

3. "Coupling LONI Institute Computational Scientists, CyberTools and Science Drivers at the Molecular Level"; PIs: Thomas Bishop (Tulane), Shantenu Jha (LSU), and Nayong Kim (LSU); LI CS: Andre Merzky (LSU) at the first stage of the project.

4. "Automated Data Archiving with PetaShare"; PIs: Tevfik Kosar (LSU), Gabrielle Allen (LSU), Sumeet Dua (LA Tech), Frank Löffler (LSU), and Erik Schnetter (LSU); LI CS: Hideki Fujioka (Tulane).

5. "Developing a High Performance Computational Biology and Material Science Lab at Southern University (HPC-BMSL)"; PIs: Ebrahim Khosravi (SUBR), Shuju Bai (SUBR), Rachel Vincent-Finley (SUBR), Shizhong Yang (SUBR); LI CS: Shizhong Yang (SUBR).

6. "Data Management for Disaster Management though PetaShare"; PIs: Ramesh Kolluru (ULL), Tevfik Kosar (LSU), Raju Gottumukkala (ULL), Rusti Liner (ULL); LI CS: Raju Gottumukkala (ULL).

7. "Application Profiling on LONI"; PIs: Erik Schnetter (LSU), Maciej Brodowicz (LSU), Steve Brandt (LSU), and Mayank Tyagi (LSU); LI CS: unassigned.

8. "Surface Plasmon Excitation in inhomogeneous metal-dielectric Composites"; PIs: Dentcho Genov (LA Tech), and Shizhong Yang (SUBR); LI CS: Shizhong Yang (SUBR).

9. “Refinement of Integral Membrane Protein Structure Predictions”; PIs: Christopher Summa (UNO), Steven Rick (UNO), and Zhiyu Zhao (UNO); LI CS: Zhiyu Zhao (UNO).

10. "Parallel-GIS: A High Performance Open Source Geospatial Analysis"; PIs: Ramesh Kolluru (ULL), Baker Kearfott (ULL), Raju Gottumukkala (ULL); LI CS: Raju Gottumukkala (ULL).

Starting on March 2010 (Y3), the scientific committee and the LI CSs approved the 2010 LI Projects, and are:

1. “Next Generation Parallel Codes for the Simulation of Correlated Materials”; PIs: M. Jarrell, J. Moreno and J. (Ram) Ramanujam, (LSU); LI CS: Tae-Woo Lee (LSU).

2. “Parallel Algorithms for Large Scale Data Clustering”; PIs: Vijay Raghavan, Ryan Benton, Raju Gottumukkala (ULL), Box Leangsuksun, (LA Tech) ; LI CS: Raju Gottumukkala (ULL).

3. “Parallel Optimization Algorithms for Disaster Management”; PIs: Ramesh Kolluru, Mark Smith, N. Raju Gottumukkala, Baker Kearfott (ULL), Dileep Sule (LA Tech) ; LI CS: Raju Gottumukkala (ULL).

4. “iLevee: Intelligent Flood Protection Monitoring, Warning and Response System”; PIs: Ramesh Kolluru, Dean Mallory, N. Raju Gottumukkala (ULL), Box Leangsuksun (LA Tech), Honggao Liu (LSU); LI CS: Raju Gottumukkala (ULL).

5. “High Performance Computational Biology and Material Science Projects at Southern University HPC-BMSL Lab (FY: 2010~2011)”; PIs: Ebrahim S. Khosravi (SUBR), Seung-Jong Park, Marcia Newcomer, Shengmin Guo (LSU), Shuju Bai, Shizhong Yang, (SUBR); LI CS: Shizhong Yang, (SUBR).

6. “Simulating Larval Dispersal in the Northern Gulf of Mexico”; PIs: Caz Taylor (Tulane), Richard Condrey (LSU), Woody Nero (NOAA), Erin Grey (Tulane), Carey Gelpi (LSU); LI CS: Hideki Fujioka (Tulane).

7. “Computational Infrastructure for Genome-wide Change Point Analysis at Basewise Resolution and Transcriptome Characterization on the Isoform Level”; PIs: Dongxiao Zhu (UNO), Zhiyu Zhao (UNO), Kun Zhang (Xavier) and Erik Flemington (Tulane); LI CS: Zhiyu Zhao (UNO).

8. “Surface plasmons in metal/semiconductor composites and devices”; PIs: Dentcho A. Genov, Abdul Khaliq (LA Tech); LI CS: Abdul Khaliq (LA Tech).

9. “Improving Antibody Design by Structure Prediction, SCOP Classification and Protein - Protein Docking”; PIs: Seth Pincus, Children's Hospital New Orleans, LSU, Zhiyu Zhao, UNO, Bin Fu, University of Texas – Pan American; LI CS: Zhiyu Zhao (UNO).

10. “Computational Model of Pulmonary Small Airway Interdependence”; PIs: Hideki Fujioka, Tulane, David Halpern, University of Alabama, and Donald P. Gaver, Tulane; LI CS: Hideki Fujioka (Tulane).

11. “Thermal Modeling and Thermo-mechanical Modeling of Thermal Barrier Coatings (TBCs) using Ansys Fluent Commercial Package”; PI: Stephen Akwaboa, (SUBR); LI CS: Shizhong Yang, (SUBR).

12. “Large-Scale First Principles Computation and Simulation of Catalytic Properties of Nitrogen Doped Carbon Nanotubes for Dioxygen Reduction”; PIs: Guang-Lin Zhao, Ebrahim Khosravi, Shizhong Yang (SUBR); LI CS: Shizhong Yang, (SUBR).

13. “Leveraging LONI Workflow Developments onto TERAGRID To Enable High Performance High Throughput Molecular Dynamics Simulation”; PI: Thomas C. Bishop (Tulane); LI CS: Hideki Fujioka (Tulane).

14. “A learning machine tool for large-scale solvers on parallel computers”; PI: Abdelkader Baggag (LA Tech); LI CS: unassigned.

Details regarding these projects are provided in appendix C, with more information in appendix B, where our LI CSs explain their research.

1.II.b) LONI Users:

Currently, there are 1031 Louisiana users with LONI accounts, of whom 185 have logged on to a LONI system in the past 6 months. (Source: The allocations database and the user directory.)

1.II.c) External Funding

Our LI Faculty have obtained numerous external funding. Up to Y3, there have been about 14 grants from National agencies, for a total of $31M. There are 13 awards from the State of Louisiana., for a total of $461K.

A great success is the Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA), a $20M award to the LI sites which will transform materials science research and education throughout the State of Louisiana. The Alliance members are: Louisiana State University (LSU, lead institution), Grambling State University (Grambling), Louisiana Tech University (LA Tech), University of New Orleans (UNO), Southern University at Baton Rouge (SUBR), Tulane University (Tulane), and Xavier University (Xavier) which is a new LI member.

A major research focus of the Alliance will be to develop common computational tools for the study of multiscale phenomena in three Science Driver areas of current strength in the State, and of substantial technological and economic importance: (1) correlated electronic materials, (2) energy materials, and (3) biomolecular materials. The project will impact education and workforce development in the State by creating a comprehensive set of programs addressing various demographic needs.

The LI CSs have also obtained funding, with 7 national awards for a total of $6M (Y1-Y3 of the project), and 5 State awards for a total of $882K.

At the moment, LI Faculty have about $9.6M in pending awards.

For more details on these awards, we refer you to appendices A and B.

Here we list the grants from other LI SIs.

Gabrielle Allen (LSU):

DOE/BOR: Ubiquitous Computing and Monitoring System (UCoMS) for Discovery and Management of Energy Resources, $3.3M (total). Allen, Co-PI at LSU. [With ULL, SUBR]

NSF OCI: The LONI Grid - Leveraging HPC Resources of the Louisiana Optical Network Initiative for Science and Engineering Research and Education, $2.2M (Total, LSU). Allen, Senior Investigator. [With LONI]

NSF OCI: Leadership-Class Scientific and Engineering Computing: Breaking Through the Limits (Blue Waters), $208M (Total), $160K (LSU). Allen, PI at LSU. [With NCSA, UIUC and RENCI]

NSF ESPCoR/BOR: Louisiana's Research Infrastructure Improvement Strategy (Includes Cyber-Tools), $12M (Total), October 2007 to September 2010, Allen, PI at LSU (subcontracts to ULL, LA TECH, Southern), Lead of CyberTools Component. [With LA TECH, ULL, SUBR]

NSF MPS: XiRel: A Next Generation Infrastructure for Numerical Relativity, $250K (Total, LSU), September 2007 to July 2010, Allen, Principal Investigator. [With RIT, Georgia Tech, AEI]

BOR PKSFI: Center of Excellence in Integrated Smart Sensor Surveillance System (CyberSpace), $3,638,000 (Total), June 2007 to June 2012, Allen, co-PI. [With LA TECH]

SURA/NOAA: SURA Coastal Ocean Observing and Prediction Program, $150K (LSU), December 2006 to August 2008, Allen, PI at LSU. [With SURA, TAMU, RENCI, UAB, VIMS, GOMOOS, UNC]

NSF CNS: MRI: Development of PetaShare: A Distributed Data Archival, Analysis and Visualization System for Data Intensive Collaborative Research, $958K, August 2006 to July 2010, Kosar, PI, Allen, co-PI. [Many partners across state]

NSF LRAC Numerical Relativity and Black Hole Mergers, Computer allocation at National Centers. Over 5,000,000 CPU hours (SUs) across various NSF sites, 2008 to 2009. Allen, co-PI. [With AEI]

B. Ramu Ramachandran (LA Tech):
Graduate Fellows in Engineering 2011-15, $200,000 (Louisiana Board of Regents) [Jim Palmer is the PI]
Graduate Fellows in Computational Analysis and Modeling 2011-15, $200,000 (Louisiana Board of Regents)

Z. Dick Greenwood (LA Tech):
NSF "Collaborative Research: Accelerating Large Hadron Collider Computing with Graphics Processing Units", Box Leangsuksun, Co-PI, $178,840.00, Pending

Pedro Derosa (LA Tech):

Project title	**Funding Source**	**Amount**	**Period**
"Multiscale Modeling of Nanocomposites"	AFRL	$353,000 (annually renewed)	12/01/2007-10/13/10
"JFAP Summer Research Program (2009)"	NSF-BoR	$20,000	05/01/09-04/30/10
"Development of a Multi-scale Tool to Study Electronic, geometrical and Conductive Properties of Polymers"	BoR	$129,871	06/01/2009-06/31/2012
"Multiscale Modeling of Thermal Transport in Electrically Active Nanocomposites",	AFRL	$65,000	08/26/09-08/26/10

"Conjugated Polymer Nanostructures for Supercapacitors and Batteries – Device Optimization and Modeling"	DoE Thorugh COES	$40,000	09/01/2009-08/31/2010

1.II.d) Publications

These publications can be cross-institution, and some of them are at the interface between biology, materials, and computational science.

During Y3, LI Faculty had 17 published publications, 9 in press, 5 submitted and 6 in progress. The LI CSs had 1 in press, and 8 published. For more details on these, we refer you to appendices A and B. LI Graduate Fellows (GFs) have 6 published, or accepted presentations (appendix D).

LI Faculty also have one book chapter and two in preparation, and one poster presentation.

From LI SIs:

Collin Wick (LA Tech):

1. Wu, H., Wick, C.D., Computational investigation on the role of plasticizers on ion conductivity in poly(ethylene oxide) LiTFSI Electrolytes (2010) Macromolecules, 43 (7), pp. 3502-3510.
2. Wick, C.D., Dang, L.X., Computational investigation of the influence of organic-aqueous interfaces on NaCl dissociation dynamics, (2010) Journal of Chemical Physics, 132 (4), art. no. 044702.
3. Sun, X., Wick, C.D., Dang, L.X., Computational studies of aqueous interfaces of SrCl2 salt solutions (2009) Journal of Physical Chemistry B, 113 (42), pp. 13993-13997.
4. Wick, C.D., Electrostatic dampening dampens the anion propensity for the air-water interface (2009) Journal of Chemical Physics, 131 (8), art. no. 084715.
5. Wick, C.D., Dang, L.X., Investigating hydroxide anion interfacial activity by classical and multistate empirical valence bond molecular dynamics simulations (2009) Journal of Physical Chemistry A, 113 (22), pp. 6356-6364.
6. Wick, C.D., Xantheas, S.S., Computational investigation of the first solvation shell structure of interfacial and bulk aqueous chloride and iodide ions (2009) Journal of Physical Chemistry B, 113 (13), pp. 4141-4145.
7. Wick, C.D., NaCl dissociation dynamics at the air-water interface (2009) Journal of Physical Chemistry C, 113 (6), pp. 2497-2502.

B. Ramu Ramachandran (LA Tech):

1. L. M. Pratt, T. Phuong, N. V. Nguỹên, and B. Ramachandran, "Halomethyllithium carbenoid cyclopropanation reactions: A computational study of the effects of solvation and aggregation," Bull. Chem. Soc. Japan 82, 1107-1125 (2009).
2. 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 (accepted, 2010).

Daniela Mainardi (LA Tech):

1. Dathar, G.K.P., Mainardi, D.S., Kinetics of hydrogen desorption in NaAlH4 and Ti-containing NaAlH4 (2010) Journal of Physical Chemistry C, 114 (17), pp. 8026-8031.
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Andrei Paun (LA Tech):
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Z. Dick Greenwood:
In 2009-10, 56 papers appeared in Physical Review D, Physical Review Letters, Physics Letters B, Nuclear Instruments and Methods in Physics Research A, and Nuclear Physics A.

1.II.e) Presentations

LI faculty gave 12 invited presentations outside the State of Louisiana until EOY3. During Y3, they had 24 presentations at local (LA) conferences, 23 at national conferences, and 4 at international conferences.

LI CSs had 5 presentations at a local level, and 6 at a national level. LI GFs also had 7 presentations.

Here are the some presentations from LI SIs:

1. B. Ramachandran, "Cyclopropanation reactions of halomethyllithium carbenoids: A computational study," B. Ramachandran and L. M. Pratt, at the Southern School of Computational Chemistry, Jackson State University, June 29, 2009
2. B. Ramachandran, "Computational Strategies for Reactions of Aggregated and Solvated Organolithium Carbenoids," B. Ramachandran, Purnima Kharidehal, and Lawrence M. Pratt, at the Southern School of Computational Chemistry, Jackson State University, April 23-24, 2010.
3. Zeno Greenwood, "High Energy Physics Experiment and Computing Grid", at the Universidade Federal do ABC, Sao Paulo, Brazil on Sep. 23, 2009. Invited colloquium.
4. Songming Hou: "Imaging using multi-frequency data", Tsinghua University, 2009
5. Songming Hou: "Interface Problems and Interface Shape Classification", University of California, Irvine, 2009
6. Songming Hou: "Shape Reconstruction and Classification", Colorado State University, 2010
7. Songming Hou: "Shape Reconstruction and Classification", Colorado School of Mines, 2010
8. Songming Hou: "Shape Reconstruction and Classification", Portland State University, 2010
9. Songming Hou: "Interface Problems and Interface Shape Classification", University of Texas, Arlington, 2010
10. Songming Hou: "Shape Reconstruction and Classification", Michigan State University, 2010

1.II.f) LI Research Impact

The metric regarding the LI research impact is having new non-LI-funded faculty working with the LI. Dr. Juana Moreno, LSU, and Dr. Amitava Jana, SUBR, continue to work with the LI. New members at ULL are Dr. Vijay Raghavan, Dr. Baker Kearfott, Dr. Azmy Ackleh, and Dr. Ryan Benton. As mentioned before, Xavier University has also become an LI member, which will bring more faculty working for the LI during out fourth year.

1.III. Economic Development Objectives, Metrics and Success Criteria

Objective	Metric	Success Criteria	Status
Student internships with companies	Number of placements	2 students placed each year; 20 total (not all will be LI-funded)	From students under the supervision of faculty associated with the LI (Sec. 1.III.a).
Pilot program with Council on Competitiveness	Program established	15 students at community college trained in CS each year, 30 total placed in companies, 10 enter universities for continued study in CS	None
Industrial partnerships	Partnerships in projects with industrial partner (any company who has joint project with LONI)	25% of total projects; 20 partners in 5 years	In progress (Sec. 1.III.b).
Industry grants	Sponsored research from companies	25 by Y5 across all sites	In progress (Sec. 1.III.b).
Centers of Excellence (UIRCs)	Number formed with multi-year duration	1 by EOY3, 3 by EOY4, 5 by EOY5, all industry-funded with at least 1 industry staff member on-site (across all LI sites)	Two proposals submitted (Sec. 1.III.c).
New companies formed	Number of new companies	1 by EOY3, 3 by EOY4, 6 by EOY5	None in Y3.

1.III.a) Students doing Internships

Some institutions have students doing internships with companies. Even though they are/were not supported by the LI, the SIs are tightly connected with the LI.

LA Tech:

* Narate Taerat (PhD/CAM; LI GF) is a visiting researcher at Sandia National Laboratory at California, working with OVIS team (http://ovis.ca.sandia.gov) during Summer 2010.
* Tyler Michalak (BS/NSE) and Travis King (BS/Biomed) were interns at AFRL during Summer 2009.
* Joshua Brown (PhD/ENGR) is on an internship at AFRL during Summer 2010.
* Ram Dhullipudi (PhD/ENGR) spent three months at the LHC in CERN, Geneva.

1.III.b) Partnership with Companies with a Joint Project with the LI

The LONI Institute **ULL** research and team is involved with the following state agencies
a. Louisiana GOHSEP (Governors' Office of Homeland Security and Emergency Preparedness)
b. Louisiana Economic Development (LED)
c. Louisiana Office of Coastal Protection and Restoration
d. Louisiana Department of Natural Resources

LA Tech:
* Network Foundation Technologies (www.niftytv.com/) is a start-up company in our incubator (with 40 employees) that has been able to grow its company in an environment with reliable access to LONI's cyberinfrastructure.
* In partnership with the Cyber Innovation Center (CIC; www.cyberinnovationcenter.org/home/) at Bossier City, Louisiana Tech has developed numerous industry partners that are collaborating with faculty on cyber security projects. LONI's computers and networks have been a major factor in attracting these partners to North Louisiana. These partnerships are expected to expand significantly as soon as LONI puts a node in the CIC facility that is nearing completion.
* The CIC has been able to use LONI as a major part of its marketing and recruitment package that has attracted federal agencies to North Louisiana, which in turn has expanded our research opportunities and industry partnerships.

UNO:
* Dr. David Mobley has a collaborative project with IBM Research Labs (Almaden, CA) and Glaxo-Smith-Kline, and another with Merck-Frosst (Canada).

1.III.c) Formation of a Center of Excellence (UIRC)

UNO: Computer Science faculty have a new Board-Approved Center, the Greater New Orleans Center for Information Assurance (GNOCIA).

ULL: A Letter of Intent was accepted by the NSF I/UCRC program with the NIMSAT Institute as the lead to establish a center of excellence for Cyberinfrastructure for Disaster Management. Another faculty member of UL Lafayette from the Center for Advanced Computing Studies (CACS), Dr. Vijay Raghavan has a n existing planning grant awarded. We have agreed to combine our projects and research areas to submit a full proposal in October 2010.

1.IV. Collaboration Objectives, Metrics and Success Criteria

Objective	Metric	Success Criteria	Status
Between computational scientists and biologists, materials	Joint papers and proposals	2 interdisciplinary papers (including preprints from a LI preprint series) per group per year; 1 at interface between bio, materials, computation per group per year; 50% of proposals have 2 of 3 disciplines	Numerous from faculty and staff associated with the LI (Sec. 1.II.c and 1.II.d).
Inter-university	Number of joint papers and proposals	2 papers, 1 proposal (including preprints from a LI preprint series) per group per year	Numerous from faculty and staff associated with the LI (Sec. 1.II.c and 1.II.d).
Inter-university	New joint projects	30 new multi-university projects proposed to SC per year	Numerous from faculty and staff associated with the LI (Sec. 1.II.a, appendices B, C)
National	Visits to national labs	3 students, 2 staff, and 6 faculty with visits to national labs per year, 2-3 each summer across all sites	From students under the supervision of faculty associated with the LI (Sec. 1.IV.a).

1.IV.a) Visits to National Labs

LI Faculty Christopher Taylor visited the Joint Genome Institute for a week long workshop on microbial genomics and metagenomics in June 2009.

Dr. Ramesh Kolluru, Executive Director of the NIMSAT Institute was invited to Sandia National Laboratories (SNL), located at Albuquerque, NM to explore collaborative R&D opportunities with the National Infrastructure Simulation and Analysis Center (NISAC). NISAC is a collaborative including Sandia National Laboratories and Los Alamos National Laboratories (LANL), in a cross-cutting partnership of the US DHS and the US DOE. A few months later, the initial exploration resulted in a follow-up meeting at the Los Alamos National Labs attended by Mr. Dean Mallory, Assistant Director of the NIMSAT Institute.

These meetings at the national labs set the foundation for a meeting hosted by the DHS Risk Modeling and Development Branch attended by SNL, LANL and the NIMSAT Institute, resulting in the launch of a partnership and a pilot project aimed at developing an analysis of the

economic impacts and disruption consequences to the Port Fourchon energy complex in Louisiana.

LA Tech:
* Collin Wick is spending a part of Summer 2010 at PNNL.
* Dick Greenwood has made multiple visits to FermiLab near Chicago, and CERN in Switzerland, where he is a part of the ATLAS collaboration conducting experiments at the Large Hadron Collider.
* Box Leangsuksun - multiple visits during the year to Oak Ridge National Laboratories.
* Neven Simicevic - multiple visits to Thomas Jefferson National Lab in Newport News, VA.
* Narate Taerat (LI GF) is a visiting researcher at Sandia National Laboratory at California, working with OVIS team (http://ovis.ca.sandia.gov) during Summer 2010.

1.IV.b) Collaborations

UNO: Some collaborations include with the University of Virginia researchers on DNA Replication, with Tulane-HSC researchers on RNA-Sequencing, and with LSU-HSC researcher on analysis of microbial diversity. Also they have projects ongoing involving collaborators at: Berkeley, UCSF, Notre Dame, LSU, and University of Virginia.

LA Tech:
* Dentcho Genov collaborates with people at LSU and SUBR.
* Dick Greenwood of the Louisiana Tech Physics Program collaborates with Tevfik Kosar in the PetaShare storage project. This work, as well as Greenwood's Grid computing work on the Dell cluster at LSU, ERIC, has facilitated the processing of 8.5 million high energy physics events during the past year.
* Sumeet Dua collaborates through LBRN and other collaborations with LSU and others.

LA Tech/LSU:
* Abdelkader Baggag, Mark Jarrell, and Juana Moreno have started collaborating.

To foster collaborations across the State of Louisiana, we will start an LI/La-SiGMA Seminar Series with speakers from the different institutions, and where each lecture is broadcast via the Access Grid to all the LI /La-SiGMAsites. Starting this fall, the series would be managed by Bhupender Thakur, the LSU LI CS. In subsequent semesters, the other LI CS should each take their turn. Suggestions for the speakers and talk titles will come from the LI researchers. Each LI site would host at least one speaker a semester.

1.V. Education and Training Objectives, Metrics and Success Criteria

Objective	Metric	Success Criteria	Status
Statewide education	HD video courses offered	4 courses per year with students from 4 universities, and 20 total students per course receiving credit.	1 HD video course and three other courses used LONI (Sec. 1.V.a).
Statewide training	Number of training workshops, people trained	Initially 2 HPC & CSs workshops offered per year, increasing to 4 by Y5; at least 50 people trained each year, 400 total	28 tutorials (346 attendees) and 8 workshops (164 attendees) offered (Sec. 1.V.b).
High school education	Summer camps	1 per year for LI members	2 Summer Camps (Sec. 1.V.c).
High school courses	Teachers offer LI-related material in courses	10 new teachers offer classes with LI material each, year starting in Y2	None yet.

1.V.a) HD Video Courses

LA Tech:
* Received "Intro to HPC" from LSU (Thomas Sterling) in Winter quarter with Box Leangsuksun as the local instructor.
* Baggag is working with Jarrell and Moreno in writing a proposal on Computational Science and Engineering education across the state of Louisiana, which will be delivered by HD video or AccessGrid technology.
* Baggag delivered a seminar at LSU which was broadcast across the State using HD video (AccessGrid).

LA Tech is also are using LONI resources for teaching a few courses on campus:

1. PHYS 510: Mathematical Methods in Physics: Fall 2009
Assignments included computations for which students were expected to use LONI computers, especially Painter.
2. MATH 587: ADVANCED SCIENTIFIC COMPUTING: Spring 2010
a. Control volume method for solving 3D unsteady state Navier-Stokes equations and simulation techniques
b. FDTD and FDFD method for 3D electromagnetic simulation
3. CHEM 424/524 Quantum Chemistry: Spring 2010
a. Matrix diagonalization (unitary transform) was used to calculate energy eigenvalues and bound state wave functions of simple one-dimensional potentials.

b. Hartree-Fock, MP2, and Density Functional Theory were used for molecular geometry optimization, vibrational frequency calculations, and for calculating potential energy curves of diatomic molecules.
c. Pure and hybrid density functionals were used to calculate reaction thermochemistry.

LSU:
LI faculty, Mark Jarrell, as part of an NSF PIRE project, taught a course entitled, "Advanced Solid State Physics". In addition to the traditional subjects, this course also covered a number of modern computational methods, such as dynamical mean field theory, quantum Monte Carlo, etc. In addition to a number of students at LSU the course was taught via asynchronous video to students in Germany and Switzerland. This course will be open to students throughout the state as part of La-SiGMA.

1.V.b) Workshops and Tutorials on HPC and Computational Sciences

The LI staff computational scientists have worked with LONI staff and its member campuses to develop and hold training workshops on the use of LONI and its advanced cyber-services, as well as annual conferences and workshops. Themes are based on overlaps between various partnerships, such as application-based workshops and tools-based workshops.
Here, we provide a list of the workshops and tutorials LONI and HPC LSU organized, as well as the number of participants. Even though we only list the events after Summer 2009, these workshops and tutorials have been offered previously as well. Many faculty, research associates, graduate and undergraduate students from across the State attended and have received training on LONI.

Semester	Training	No. Enrolled
	Workshops	
Summer 2009		
June, 15-18	Beowulf Summer Camp	22
July, 5-11	SC09 Parallel & Distributed Computing	32
Aug., 3-7	GLC Petatscale Workshop	18
Summer 2009	Total	72
Summary	**72 people were trained in Summer 2009 in 3 workshops.**	

Semester	Training	No. Enrolled
	Tutorials	
Fall 2009		
Sep. 1, 2, 8	Introduction to Linux	31
3-Sep	Welcome to HPC	27
24-Sep	Introduction to MPI	12
10-Sep	Allocations and Accounts	12
15-Sep	Introduction to Vi	10
21-Sep	Advanced Linux	13
17-Sep	Job Management with PBS & LoadLeveler	11

28-Sep	Introduction to LaTex	8
1-Oct	MPI Part 2	9
15-Oct	Introduction to Gaussian	23
19-Oct	Introduction to Cactus	5
22-Oct	Introduction to OpenMP	7
29-Oct	OpenMP Part 2	5
5-Nov	Python for HPC	28
12-Nov	Introduction to HPC Visualization	10
3-Dec	Introduction to Globus	7
Fall 2009	Total	218
	Workshops	
October, 6-7	LONI HPC Workshop, at LA Tech	20
October, 26-27	LONI HPC Workshop at ULL	31
Fall 2009	Total	51
Summary	**218 people were trained in Fall 2009 in 16 tutorials and 51 people attended 2 workshops.**	

Semester	Training	No. Enrolled
	Tutorials	
Spring 2010		
28-Jan	Introduction to HPC at LONI & LSU	10
4-Feb	Account & Allocation Management	10
11-Feb	Job Management	12
3-Mar	Introduction to MPI	6
11-Feb	MPI part 2	2
18-Mar	Molecular Dynamics	4
25-Mar	MPI/OpenMP Hybrid Programming	2
26-Mar	Introduction to C++	32
15-Apr	Introduction to Ruby	14
11-Apr	Introduction to Cactus	18
29-Apr	Introduction to CPMD	6
5-May	Profiling with TAU	12
Spring 2010	Total	128
	Workshops	
March, 26-27	CCT/LBRN/LI Workshop on Computational Biology	14
March, 29-30	LONI HPC Workshop at UNO	12
April, 28-29	LONI HPC Workshop at LSU	15
Spring 2010	Total	41
Summary	**128 people were trained in Spring 2010 in 12 tutorials, and more than 41 people attended 3 workshops**	

LONI High Performance Computing Workshops covered an overview of HPC environment of IBM Power5 and Linux machines at LONI, basic AIX/Linux operating system commands and editors, introduction to Parallel Computing, introduction to MPI and advanced MPI, introduction to programming with OpenMP, and the LONI Portal.

Other workshops by LI Faculty include,
Baggag, "High-Performance Computing and Large-Scale Numerical Modeling," one week course at Pole Universitaire Leonard De Vinci, Paris, France, March 15-19, 2010.

1.V.c) Summer Camps involving High School Education

ULL:
The Louisiana Immersive Technologies Enterprise (LITE), one of the LI collaborators is offering a high school summer internship program, encouraging the early adoption of computing and visualization in STEM education.

LA Tech:
For the 2009 JFAP Summer Outreach program (Derosa PI), one of the interns was Mr. Christopher Akers, a high school student that worked with Dr. John Shaw in the Physics Department.

LSU/SUBR:
Bety Rodriguez-Milla (LI, Scientific Coordinator), Rachel Vincent-Finley (LI Faculty, SUBR), and Kathryn Traxler (LSU) received an award from the Louisiana Board of Regents titled "Computational Science Workshop for Louisiana Educators." The award is in the amount of $29,726, and will fund a one week summer workshop taking place at CCT July 19-23, 2010. The workshop's goal is to guide Louisiana high school teachers in how to incorporate computational science into their curricula.

LSU:
SI Sterling continues to host the summer Beowulf Boot Camp for High School Students & Teachers. During the week-long boot camp, the students learn how to use supercomputers for research, develop and run basic applications and experiment with computer science techniques.

1.V.d) Other Outreach Activities

CCT faculty Juana Moreno, Department of Physics & Astronomy, and LI SI Gabrielle Allen, Department of Computer Science, worked with CCT staff Bety Rodriguez-Milla (LI Scientific Coordinator) and Kathy Traxler to secure funding from the National Science Foundation and the Louisiana Board of Regents for a Research Experience for Undergraduates (REU) summer program on "Interdisciplinary Research Experience in Computational Sciences." During this program, 17 college students from Puerto Rico, Illinois, Ohio, New York, Florida, Arkansas, Missouri, Michigan, Pennsylvania and Louisiana will collaborate with CCT faculty and staff on advanced computational research projects. LI members Gabrielle Allen, Juana Moreno, Mark

Jarrell are all participating in the program as mentors. Moreno and Jarrell's group has four REU students who are working on using GPUs to accelerate the inner loops of our calculations. They have achieved a speedup of roughly 70 times in some codes essential to our effort. These codes will also allow us to use heterogeneous machines that are now becoming available at ORNL and through the NSF TeraGrid.

3. CONTRIBUTIONS

The LI is now coming to a completion personnel-wise. We are now on a second year for some of the LI Faculty, and they have already generated publications, presentations, and external funding.

3.I. Contributions to the state research and education capacity.

LI Faculty, LI CSs have all contributed to the state research and education capacity. There is the potential to teach novel and specialized courses across the LI via the access grid (AG). In the same way, the LI/La-SiGMA will have a Seminar Series starting on Fall 2010 where all the LI/ La-SiGMA institutions will participate synchronously via AG.

LI CSs have also participated during LONI-HPC training as local instructors. We have started supporting 2 graduate students per site in Y3 (although we had 9 this year).

As shown on the appendices there are numerous publications and presentations from both the LI Faculty and LI CSs.

Another great addition was the new LI membership of Xavier University. Xavier University is the only NSF Center of Excellence in the state, and the most successful HBCU in the nation.

Other LI people are also involved in education, outreach and training for high school and undergraduate students, such as Sterling's Beowulf booth camp, and Moreno and Allen's REU program.

3.II. Securing external federal and private sector funding.

LI Faculty and LI CSs have obtained funding from State and Federal agencies. The new NSF-ESPCoR RII was LI-led and is the largest award ever received in the State of Louisiana ($20M). The total amount of awards for the LI funded people is about $37M, with about $9M in pending awards. Both HPCOPS and La-SiGMA will be supporting staff members.

3.III. Infrastructure.

The current and the new NSF-EPSCoR awards are and will be providing advanced CI for the entire state. The CyberTools project will also play an important part in the La-SiGMA project. The NSF HPCOPS project keeps connecting the LONI infrastructure to the TeraGrid, which is the NSF's national backbone for advanced CI

3.IV. Economic Development.

As described above, corporate partnerships are being explored, with companies such as GeoComp Corporation, PB Americas, Shannon & Wilson, James Lee Witt Associates, SMARTEC and TIE Technologies.

4. PROJECT REVISIONS.

We do not expect any revisions to the project deliverables. We expect to continue on track to deliver what was originally promised, even after two changes of PIs. However, with the budget cuts and the hiring freezes, LSU might use the unspent money to hire more graduate fellows and potentially start at postdoctoral fellowship at LSU.

Appendix A

LI Faculty White Papers

White Paper for Abdelkader Baggag, Associate Professor of Computer Science, LA Tech University

LI FACULTY (September 2008 – present)

Abdelkader Baggag, PhD

Associate Professor of Computer Science
Louisiana Tech University, Department of Computer Science
600 West Arizona, Nethken 149, Ruston LA 71272
Phone: (318) 257-2147, Fax: (318) 257-4922
Email: abaggag@latech.edu

EXPERTISE

Parallel numerical algorithms for large scale engineering applications and their efficient implementation on massively parallel computers.

RESEARCH INTERESTS

With academic background in computer science, applied mathematics, and engineering, and exposure to industrial and US national laboratory applications, such as NASA Langley Research Center (LaRC), I work at the interface between the numerical solution of partial differential equations, science and engineering applications, and parallel computing. I have experience, gained in particular by interacting with NASA scientists, in the numerical simulation of many disciplines such as (parallel) computational aero-acoustics (CAA), and (parallel) computational fluid dynamics (CFD): modeling the physical processes, designing and analyzing iterative algorithms, and implementing them on advanced massively parallel computers, using the message passing paradigm.

I have developed a comprehensive curriculum in HPC, and my goal is to use my prior expertise in curriculum development to set up a similar set of HPC courses within the LONI Institute.

RESEARCH GROUP MEMBERS

1. Chokchai (Box) Leangsuksun, Associate Professor, Computer Science
2. James Elliott, PhD Student, Computer Science
3. Supada Laosooksathit, PhD Student, Computer Science
4. Timothy Lindsay, Master's Student, Computer Science
5. Moayad Almohaishi, Master's Student, Computer Science

ASSOCIATE GROUP MEMBER

1. Dick Greenwood, Associate Professor, Physics

RESEARCH PROJECTS

1. Parallel Algebraic Multigrid Methods on Distributed Memory Computers
2. GPGPUs: Toward Latency Hiding

3. Porting the particulate flows code, and changing it to handle new physics, namely the simulation of the blood
4. General Purpose Graphics Processor Units and High Energy Physics (with Greenwood and Leangsuksun)

RESEARCH PROPOSALS:

1. RCS Proposal: "Parallel algebraic multigrid methods for large-scale problems on the LONI infrastructure and for the next generation of hyper-parallel platforms." **PI, submitted.**
2. LONI Proposal: "A learning machine tool for large-scale solvers on parallel computers." **PI, submitted.**
3. IARPA Proposal: "Contained Automated Software Environment." **Co-PI, submitted**
4. CDI Proposal: "Efficient parallel dimension reduction techniques for large-scale datasets in data mining." **PI,** (not submitted due to time constraints), **to be submitted in a different program.**
5. CAREER: "Accurate and scalable low-cost methods for large-scale industrial problems." **PI, to be submitted in summer 2010.**

FUTURE PROPOSALS:

1. I have been discussing with Dr. Dai on the development of a research proposal to be submitted to the NSF Computational Mathematics Program. I will be the PI. This is still in the making. We are testing the idea on an existing code. The proposal will be submitted late August/early September.
2. I am also outlining a grant proposal with Box on GPGPUs. We have already published a paper together, and I will be writing another paper with one of the students. The details of the proposal will be on "linear algebra, GPGPUs, latency hiding and check-pointing".
3. These proposals will naturally lead to a multi-disciplinary research proposal which will be submitted to NSF under the PetaApps program, which is yet to be opened. I am preparing the material and the collaboration for such an ambitious program.

RESEARCH PROJECT 1:

PARALLEL ALGEBRAIC MULTIGRID METHODS ON DISTRIBUTED MEMORY COMPUTERS FOR LARGE-SCALE INDUSTRIAL APPLICATIONS

Massively parallel computer systems, incorporating thousands of processors, are becoming a reality in Louisiana, through the LONI institute. Thus, one can hope that we are now able to test more detailed mathematical models with millions of degrees of freedom. Massively parallel computing is a major way to analyze many challenging problems in engineering, and offers a more flexible and scalable approach than experimentation. This, however, places a heavy burden on the design of suitable algorithms, their efficient implementation on parallel architectures and the development and maintenance of very large software.

The fast and efficient solution of linear systems of equations is a key task in the process of many industrial problems, as it represents more than 90% of the computational time. It is therefore necessary to develop algorithms of *optimal complexity* where both memory and compute time should depend only linearly on the problem size. Moreover, the increasing demands of computationally challenging applications on complex geometries, which run on high-performance computers with tens or hundreds of thousands of processors, have necessitated the development of *scalable solvers and preconditioners*.

One of the most effective ways to achieve *scalability* is the use of multilevel techniques. Algebraic multigrid (AMG) methods have proved to be efficient algorithms for solving large linear systems on *unstructured grids*. By the term "algebraic multigrid," we mean the class of solvers based on multigrid principles, but which do not depend on the availability of the underlying mesh about the problem. AMG methods use only the information available in the linear system of equations, and therefore are of special interest especially for unstructured grids where no hierarchy of meshes is provided, e.g. in finite element discretizations.

The first aim of the proposed project is to efficiently implement the (sequential) Ruge-Stüben classical AMG algorithm, and extensively test it on real life engineering applications. The second aim is to investigate new parallel approaches suitable for distributed memory computers, and implement a general parallel algebraic multigrid algorithm for finite element discretizations based on domain decomposition ideas. In particular, different parallel strategies for the coarsening phase and the smoothing operator will be examined. As for the robustness of the algorithm, an adaptive process will be utilized.

While the AMG algorithm works well for a wide range of problems, there are situations in which it requires special care, e.g., on stretched grids where obtaining a robust and efficient solution still remains problematic. One reason for this is that, sometimes, the interpolation operator does not interpolate adequately the smooth modes of the error. *Hence, a characterization of the smooth error will be provided, analyzed and implemented along the lines of element-based algebraic multigrids (AMGe), and element-free AMGe. Lastly, a careful analysis and (implementation) of the compatible relaxation algorithm, will be undertaken, as it holds much promise for parallel computation.*

The project will provide significant training of highly qualified personnel at the Masters and PhD levels. The outcome of the current project will be the development of efficient and robust parallel algebraic multigrid algorithms which scale both with machine and problem size, and an object-oriented software that is portable, modular and MPI-based.

RESEARCH PROJECT 2:

GPGPUS: TOWARD LATENCY HIDING

Abstract: In multithreaded programming on GPUs, data transfer between CPU and GPUs is a major impendence that prevents GPU to achieve its potential. Hence, stream management framework – a latency hiding strategy introduced by CUDA, becomes our attention. Streaming allows overlapping between kernel execution time and transfer time of independent data between CPU and GPUs. For this reason, the total execution time can potentially be reduced. In this project, we introduce performance models in order to study the utilization of streams. Moreover, we study two methods that are used for timing operations in CUDA, namely CUDA calls and CUDA events. CUDA call functions are functions implemented in C++, while CUDA events method is an API. Our finding shows that CUDA events method is more accurate for timing operations than CUDA call functions

Description: Due to the rapid increase in computational performance required to handle massive data sets, Graphic Processing Units (GPUs), which were first designed for specific graphics computation, have been used for non-graphics applications. This process is known as GPGPU, or General Purpose Computation using GPUs. GPUs are specialized for compute intensive, highly parallel computation via several

multithreaded processors. As such, GPUs are commonly classified as a collection of many-core Central Processing Units (CPUs). Today, GPUs have been exploited in many application areas including oil exploration, scientific data processing, and stock options pricing determination. The operations driving these applications require efficient data management and the processing of massive data sets, such that these operations can be simultaneously performed in an extremely fast fashion. However, data transfer from host to GPU devices and back slows down the application executions. To fulfill these requirements, a latency hiding strategy is needed. Due to its coprocessor status, the kernel grid aboard the GPU is invoked by a program running on CPU, which in turn distributes thread blocks of the grid to the multiprocessors. Each thread of a thread block concurrently executes its instructions on one multiprocessor. New blocks are launched on the multiprocessors again as previous thread blocks terminate. Even though the cost of each memory copy between the CPU (host) and GPU (device) is relatively very low, the millions of bytes of data and thousands of transfers of each chunk of this data required by applications can multiply those costs and lead to exceptionally high values. To reduce these costs, the GPU allows for the applications to be managed concurrency through streams. Unlike stream processing – a technique to operate on streams or sequences of data, streaming is a latency hiding strategy which allows for sequences of operations to execute successively. Different streams execute particular operations in parallel. With streams, the kernel launches the current operation and copies the memory chunk of the next operation asynchronously. In this paper we focus on memory transfer between main memory which works with the CPU and the global memory of the GPU. The internal memory transfer of the GPU (between global memory and shared memory which works directly with threads) will be the scope of another project. Besides the streaming technique, we also study two methods for timing operations in CUDA, namely CUDA call functions and CUDA events. CUDA call functions are implemented in C++ and provided in CUDA SDK. CUDA events method is an API and has to be implemented with stream.

BOOKS IN PROGRESS:

1. "An Introduction to the Finite Element Method" by Weizhong Dai, Abdelkader Baggag, Abdul Khaliq and Raja Nassar

   → I have been invited by Dr. Dai to participate as a co-author, and write the part related to parallel implementation, discontinuous Galerkin and linear system solvers. I have been working on this part since January 2010. The idea is to publish this book and use it as a textbook in a sequence of CAM courses, one will be taught by Dr. Dai and I teach the second part.
2. "Parallel Algorithms and Applications" by Abdelkader Baggag

   → This is an ongoing project since last year.

COURSE DEVELOPMENT:

"High Performance Computing and large Scale Numerical Modeling"
In this course, I will be teaching the essence of what is needed for researchers to take advantage of the machines' power, and I will spend an extra effort to hold the researchers' hand in parallelizing, debugging and optimizing some of their respective codes. The scaling of parallel algorithms has not yet matched peak speed, and the programming burden for parallel machines remains heavy.

Hence the applications must be programmed to exploit parallelism in the most efficient way possible. Today, the responsibility for achieving the vision of scalable parallelism remains in the hands of the

application developers. This course illustrates the state-of-the-art of parallel computing, and links theory to applications, through demonstrations and training.

This course should be of interest to engineers, programmers and code developers. As a first step, I will include it as part of the CAM program, and as a follow up step, I will deliver it to LONI scientists.

PEER REVIEWED PUBLICATION

1. S. Laosooksathit, C. Leangsuksun, A. Baggag, C. Chandler, "Stream Experiments: Toward Latency Hiding in GPGPU," accepted
2. Baggag, "A preconditioned scheme for nonsymmetric saddle-point problems," submitted to SIAM Journal on Matrix Analysis
3. I am a member of a research group on GPGPUs with Box. I am working on a paper with Moayad Almohaishi (master's student) and Box. The topic is on performance issues on GPGPUs. A Monte Carlo code from the physics people at UTA (Univ. of Texas at Arlington), namely Prof. Amir Farbin, has been ported on GPUs, and some optimization techniques will be explored and added to get the best performance possible from GPUs.

RECRUITMENT OF A PHD STUDENT

I succeeded in attracting Mr. James Elliott to be my Ph.D. student. He is working under my supervision, and the research topic is: "Parallel algebraic multigrid methods for large-scale problems on the LONI infrastructure and for the next generation of hyper-parallel platforms."

He has submitted his program of study to the graduate school, under the CAM program, and is successfully progressing in his research. He has already made a presentation, and he will present at the NSF annual meeting in DC in March 26, 2010.

He was awarded the LI fellowship in early June 2010.

PRESENTATIONS AND CONFERENCES

1. Baggag, "A preconditioned scheme for nonsymmetric saddle-point problems," LONI Institute, March 10, 2010.
2. J. Elliott, A. Baggag, "Parallel Computational Methods for Next Generation Computing Hardware", 87th Annual Mathematics Association of America (MAA), Section Meeting, March 6, 2010.
3. J. Elliott, A. Baggag, "Parallel algebraic multigrid methods for large-scale problems on the next generation of hyper-parallel platforms," NSF Annual Meeting, invited poster session, Washington, D.C., March 26, 2010.
4. I am invited to make a presentation at LSU on "Parallelism and large-scale linear systems," April 15-16, 2010. This presentation will be broadcast to other researchers affiliated with the LONI Institute.
5. I attended the Supercomputing Conference SC'09 in Portland, OR, November 2009.
6. I attended the "Mardi-Gras Conference on Computational Materials," March 11-14, 2010.

INTERNATIONAL VISIBILITY:

1. Pole Universitaire Leonard De Vinci, Paris, France. I have been selected to teach a one-week graduate course on "High-Performance Computing and Large-Scale Numerical Modeling," March 15-19, 2010.

TEACHING AT LOUISIANA TECH UNIVERSITY (LECTURER AND INSTRUCTOR)

CSC 220 "Data Structures"
CSC 581 "Parallel Algorithms"

Committee for PhD and Masters:

- James Elliott, PhD student. Main advisor: A. Baggag
- Lisa James, PhD student. Main advisor: K. Evans
- Scarlett Bracey, PhD student. Main advisor: K. Evans
- Halpreet, PhD student. Main advisor: S. Dua
- Supada Laosooksathit, PhD student. Main advisor: Box
- And many other students at the Masters level.

White Paper for Scott M. Duke-Sylvester, Assistant Professor of Biology, University of Louisiana at Lafayette

LI Faculty (August 2009 to present)
UL Lafayette Faculty (August 2009 to present)

Scott M. Duke-Sylvester, PhD

Assistant Professor of Biology
University of Louisiana at Lafayette, Department of Biology
300 E. St. Mary Blvd, Billeaud Hall 141
Lafayette, LA 705040-2451
Phone: (337) 482-5304, Fax: (337) 482-5834
Email: smd3729@louisiana.edu

Expertise

The application of high performance computing and mathematical algorithms to landscape ecology.

Research Interests

I am a theoretical ecologist by training and much of my research applies mathematical techniques to reveal the mechanisms driving contemporary patterns of species distribution and abundance. My current research focuses on the ecology and evolution of infectious diseases. The study of infectious diseases has emerged as an important and productive area for ecological and evolutionary research. Infectious diseases exhibit a wide range of interactions with their hosts and their study touches on many of the most basic and important ecological and evolutionary processes. Through the study of infectious diseases many important and interesting patterns and processes have been revealed. Examples of topics I am currently researching include the sources of periodic cycles in outbreak of infectious disease, the landscape ecology of diseases spread and the interaction between ecological and evolutionary processes that govern infectious disease dynamics.

My approach to research is strongly interdisciplinary and I make extensive use of both mathematical and computational modeling approaches. Modeling is a powerful tool for teasing apart the contribution of different mechanisms governing the spread of infectious diseases. I apply models to explore alternative hypotheses describing the origins of ecological and evolutionary patterns. I then use the theoretical results to design future experiments to support or falsify these hypotheses.

Research Projects

1. Revealing signatures embedded within a viral phylogeny produced by the demography of host/pathogen interactions.
2. The landscape ecology of coastal and wetland ecosystem of the southeastern United States.

Research Project 1:

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.

Research Project 2:

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 an 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. (in review). Strong seasonality produces spatial asynchrony in the outbreak of infectious diseases. *Journal of the Royal Society Interfaces*

Presentations/Talks

November 2009. Strong seasonality produces spatial asynchrony in the outbreak of infectious diseases. Department of Mathematics, University of Louisiana at Lafayette, Lafayette, LA.

March 2010. Linking the Evolutionary and Ecological Dynamics of Infectious Diseases. Department of Biology, Emory University, Atlanta, GA.

May 2010. Short-term visitor. National Institute for Mathematical and Biological Synthesis (NIMBioS), Knoxville, TN.

Grant Proposals Pending

1. Louisiana Office of Coastal Protection and Restoration.
Title: Vegetation Module for Louisiana Coastal Protection and Restoration Master Plan.
Funds Requests: $148,400 Date submitted: June 7, 2010.

Electromagnetic Metamaterials and Nanophotonics

LI FACULTY (09.2008 - present)

Dentcho A. Genov, PhD

Assistant Professor of Physics & Electrical Engineering
Louisiana Tech University, Engineering Annex, Room 220
599 W Arizona Ave, Ruston LA 71272
Phone: (318) 257-4190, Fax: (318) 257-2777
Webpage: http://www.phys.latech.edu/~dgenov/

RESERCH 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

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)

Projects Description: 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 30 papers in top peer reviewed scientific journals, including; *Nature*, *Nature Photonics*, *Nature Physics*, *Physical Review Letters*, est.. Currently my group is pursuing 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 100THz 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.

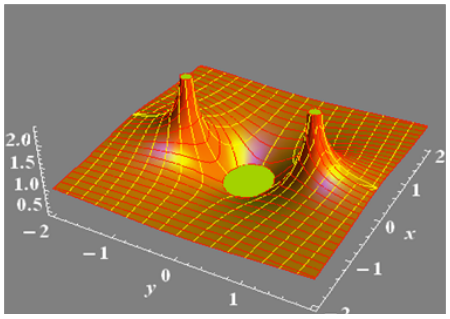

Figure 1 Electromagnetic invisibility. Any light ray that approaches the object (green circle) from the bottom, curves around it and at infinity behaves as if it has propagated trough free space. The refraction index that provides such behavior is depicted by the surface plot.

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 (see Fig. 1) 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 'memoization' 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) (Fig. 2a) 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 (Fig. 2b). 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.

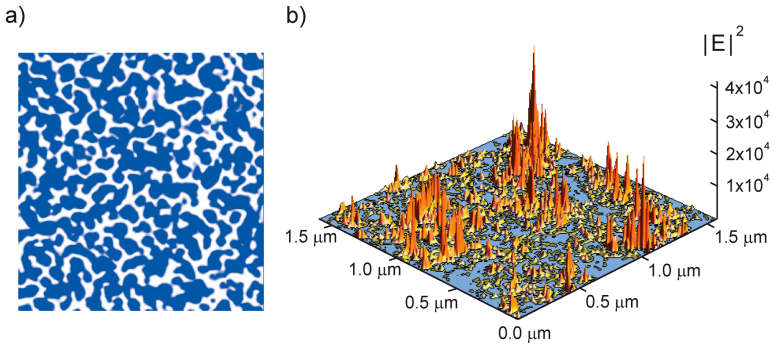

Figure 2. (**a**) Metal-dielectric composites support morphology dependent surface plasmon (SP) resonances characterized by (**b**) highly enhanced local field densities over wide frequency range[3].

d. Surface Plasmon based 100THz 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 will be identified and a prototype will be tested in the Institute for Micromanufacturing (LA Tech).

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.

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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).

Grant Proposals Pending:

1. Proposal Title: "Artificial optical materials for molding the flow of light": Louisiana Board of Regents Support Fund – (RCS) – pending funding ($138,795).
2. "PNA Substrates for Surface Enhanced Raman Scattering Sensing", DOD STTR – pending funding ($50,000).

Grant Proposals Approved:

1. Proposal Title: "Surface Plasma Enhanced Solar Cell (SPESC) ": DOE RFP ($99,982) Date awarded: 06.04.2009.
2. Proposal Title: "Optical Attractors and Continuous Index Photon Traps", LOUISIANA EPSCoR (PFUND FY2009-10) ($10,000) Date awarded: 01.04.2010.

Peer previewed publications acknowledging the LONI Institute:

1. D. A. Genov, S. Zhang, and X. Zhang, "Mimicking celestial mechanics in metamaterials", *Nature Physics* **5**, 687 (2009).

Seminars and Conference Presentations:

1. "*Electromagnetic Properties of Complex Metamaterials: from Near Field Imaging with Super Resolution to Mimicking Celestial Phenomenon in the Lab*",
Progress in Electromagnetics Research Symposium (PIERS), Moscow, Russia, August 18-21 (2009).
2. "*Controlling light with Electromagnetic Metamaterials*", LONI HPC Workshop, Louisiana Tech University, Ruston, LA, October 7, 2009.
3."*Controlling light with Artificial Optical Materials*", CAM Seminar Series, Louisiana Tech University, Ruston, LA, October 8, 2009.
4. "*Artificial Optical Materials molding the flow of light*", Physics Seminar Series, Louisiana Tech University, Ruston, LA, October 22, 2009.
5. "*Surface Plasmon Enhanced Solar Cell*", Louisiana Tech Energy Systems Conference, Shreveport, Louisiana, November 5 (2009) (Invited talk).

6. "*Controlling light with Artificial Optical Materials*", The LONI Institute All-Hands Meeting, Baton Rouge, LA, February 10, 2010.
7. "*Molding the flow of light with Artificial Optical Materials*", Mardi Gras Conference- Computational Materials and methods, Baton Rouge, Louisiana, February 11-14 (2010) (Invited talk).
8. "*Controlling light with Artificial Optical Materials*", IfM Seminar, Louisiana Tech University, Ruston, LA, March 26, 2010.

Teaching at Louisiana Tech University:

Lecturer:

ENGR592/PHYS540/PHYS470s (Computational Methods)
ELEN411/ PHYS407 (Electric and Magnetic Fields)
PHYS511/ ELEN512 (Electromagnetic Theory)
PHYS205 (Conceptual Physics I)
PHYS409 (Magnetism Lab)

White Paper for Mark Jarrell, Professor of Physics and Astronomy, LSU

Group Members (Computation and Theory of Strongly Correlated Materials)
M Jarrell, Professor
J. Moreno, Assistant Professor
C. Slezak, Visiting Proffessor
D. Galanakas, Postdoc
S. Su, Postdoc
Z. Xu, Postdoc
V. Rousseau, Postdoc
M. Nili, Student
H. Fotso, Student,
P. Reis, Student
S. Yang, Student
K. Chen, Student
Kalani Hettiarachchilage, Student
Ricky Nelson, Student
David Poliakoff, undergraduate, and REU Student
Jonathan Gluck, REU Student
Jitu Das, REU Student
Brittany Shannon, REU Student
D. Norman, Administrative Assistant

Research

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 materilas. 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)[16,17] and its cluster extensions, including the Dynamical Cluster Approximation (DCA)[18-21] 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)[22-24] simulation while disorder can be included by averaging over configurations. [18-20] 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.[25] 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.[26,27] 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[28-32] 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 which is used to treat correlations on the longest length scales.

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.[27,33]

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)[11] 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.

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 which 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 program, we teach a complete set of courses in Computational materials Science which are broadcast via interactive synchronous video to 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):

- N.S.Vidhyadhiraja, A.Macridin, C.Sen, M.Jarrell, Michael Ma Quantum Critical Point at Finite Doping in the 2D Hubbard Model: A Dynamical Cluster Quantum Monte Carlo Study , Phys. Rev. Lett., 102, 206407 .
- E. Khatami, A. Macridin, M. Jarrell The validity of the spin-susceptibility "glue" approximation for pairing in a two-dimensional Hubbard model , Phys. Rev. B,
- Karlis Mikelsons, Alexandru Macridin, Mark Jarrell The relationship between Hirsch-Fye and weak coupling diagrammatic Quantum Monte Carlo methods , Phys. Rev. E 79, 057701 (2009), arXiv:0903.0559.

- C. N. Varney, C.-R. Lee, Z. J. Bai, S. Chiesa, M. Jarrell, R. T. Scalettar High Precision Quantum Monte Carlo Study of the 2D Fermion Hubbard Model , Phys. Rev. B 80, 075116 (2009), arXiv:0903.2519.
- E. Khatami, C. R. Lee, Z. J. Bai, R. T. Scalettar, M. Jarrell Dynamical Mean Field Theory Cluster Solver with Linear Scaling in Inverse Temperature , Phys. Rev. B, 81, 201101, arXiv:0904.1239.
- S. X. Yang, H. Fotso, J. Liu, T. A. Maier, K. Tomko, E. F. D'Azevedo, R. T. Scalettar, T. Pruschke, M. Jarrell Parquet approximation for the 4x4 Hubbard cluster , Phys. Rev. E, 80, 046706.
- K. Mikelsons, E. Khatami, D. Galanakis, A. Macridin, J. Moreno, M. Jarrell Thermodynamics of the Quantum Critical Point at Finite Doping in the 2D Hubbard Model: A Dynamical Cluster Approximation Study , Phys. Rev. B, 80, 140505, arXiv:arXiv:0909.0498.
- A. K. McMahan, R. T. Scalettar, M. Jarrell The screening of 4f moments and delocalization in the compressed light rare earths , Phys. Rev. B, 80, 235105, arXiv:arXiv:0909.0539.
- 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, 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, 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, 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., Comment in press, 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, 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$_{x}$As , Phys. Rev. Lett., 104, 037201, arXiv:arXiv:1001.1716.

Recent Presentations and Talks (2009 – 2010):

- Massively Parallel and Multi-Scale Simulations of Strongly Correlated Electronic Systems. , Invited Talk, March 4, 2009, Michael Dewar Memorial Symposium: Advancing Computational Chemistry Through High Performance Computing, from the Workstation to the Petascale and Beyond. March Meeting of the American Chemical Society. Salt Lake City, Utah.
- Massively Parallel and Multi-Scale Simulations of Strongly Correlated Electronic Systems. , Keynote Lecture, The International Conference on Computational Science 2009 May 25 - 27, 2009, in Baton Rouge, Louisiana
- Quantum Criticality in a Doped 2D Hubbard Model, Invited talk, July, 21, 2009, KITP Program: The Physics of Higher Temperature Superconductivity (June 15 - September 11, 2009) Coordinators: Malcolm R. Beasley, Eduardo H. Fradkin, Douglas J. Scalapino.

- What's under the superconducting dome in the two-dimensional Hubbard model?, Colloquium, Tulane University, 9/8/09.
- What's under the superconducting dome of the two-dimensional Hubbard model?, Presented as an invited talk Wednesday, September 16th at the workshop, International Workshop on Frontiers in Density Functional Theory, September 13-17, 2009, Montauk Yacht Club, Long Island, New York
- Quantum Criticality at finite doping in the 2D Hubbard model, presented September 28 2009 as an invited talk at the workshop Recent Developments in Dynamical Mean Field Theory, September 28-30, ETH Zurich.
- 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.

External Funding:

- *Simulations of Strongly Correlated Electronic Materials*, DMR-0706379, $375,000 over the three-year period 09/01/07-08/30/10 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:

Search Results

Proposal	PI Name	Deadline	Amount Requested	Status
36341 - 1	Liu, Honggao	05/03/2010	$2,984,123.00	Submitted
	Sponsor: Board of Regents - BOR		*Type:* New	
			Date Approved: 05/03/2010	

Project Title: Bridging to XD - Leveraging the Louisiana Optical Network Initiative HPC Resources for Scientific Research and Education
Proposal Specialist:Award Specialist:
Williams, Rhonda Meyers

	Jarrell, Mark	10/15/2009	$9,123,947.00	Submitted
	Sponsor: Board of Regents - BOR		*Type:* New	
			Date Approved: 10/15/2009	
35612 - 1	*Project Title:* Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA): Leveraging Next Generation Supercomputing for the Study of Complex Multiscale Phenomena in Materials			
	Proposal Specialist:Award Specialist:			
	Young, Shirley Langford			
	Jarrell, Mark	05/28/2009	$294,936.00	Submitted
	Sponsor: Ohio Supercomputer Center (OSC)		*Type:* New	
			Date Approved: 05/26/2009	
34971 - 1	*Project Title:* Improving Developer Productivity for HPC through Cyberinfrastructure: Applications, Languages, Tools and Services			
	Proposal Specialist:Award Specialist:			
	Young, Shirley Langford			
	Jarrell, Mark	04/30/2009	$20,000,000.00	Submitted
	Sponsor: Board of Regents - BOR		*Type:* Preproposal/NOI	
			Date Approved: 04/29/2009	
34891 - 1	*Project Title:* Louisiana Graduate Research and Education Program in Computational Materials Science			
	Proposal Specialist:Award Specialist:			
	Williams, Rhonda Meyers			
	Hall, Randall W	04/20/2009	$10,000.00	Submitted
	Sponsor: Board of Regents - BOR		*Type:* New	
			Date Approved: 04/20/2009	
34809 - 1	*Project Title:* Planning for LONI Institute s Proposal to the 2009 Louisiana EPSCoR RII Competition			
	Proposal Specialist:Award Specialist:			
	Hakes, Jonathan			
34579 - 2	Jarrell, Mark	01/27/2010	$884,509.00	Submitted
	Sponsor: Dept of Energy - DOE		*Type:* Revision	

Date Approved: 01/26/2010

Project Title: Next Generation Multi-Scale Quantum Simulation Software for Strongly Correlated Materials

Proposal *Specialist:Award Specialist:*
Impson, Dana Tuminello

* Note that the La-SiGMA grant has been approved, there is also a new CMSN award that will be funded.

2010 ANNUAL REPORT FOR THE LONI INSTITUTE GRANT

Damir B. Khismatullin
Department of Biomedical Engineering
Tulane University, New Orleans, LA 70118

Postdoctoral researchers (2009 - current):
Weixiong Wang

Graduate students (2009-current):
Hongzhi Lan
Chong Chen
Yuan Teng

Undergraduate students (2009-current):
Theodore Brown, Marisa Belaidi
Andrew Kronfol (REU), Lydia Barrett (REU)

Specialization:
Computational modeling and experiments

Research fields:

1) Bio-fluid mechanics and cellular biomechanics;
2) Cell-cell interactions in inflammation, atherosclerosis, and thrombosis;
3) Medical ultrasound and biomedical applications of gas microbubbles;
4) Multiphase flows and non-Newtonian fluid mechanics

I started my appointment as Associate Professor of Biomedical Engineering at Tulane University, with 50% support from the LONI Institute Grant, in August 2008. During the third year of the grant period (August 2009 - June 2010), research in my laboratory was focused upon the following projects.

Project 1: Quantitative Biomechanical Models of Cellular Interactions with Applications in Inflammation, Atherosclerosis, and Thrombosis The goal of this project is to develop and experimentally validate computational models for the adhesive interaction of white blood cells and platelets with endothelial cells under pathophysiological conditions such as inflammation, atherosclerosis and thrombosis. The models to be developed will be an invaluable tool to explore the causes of and therapies for these diseases. My laboratory conducts both theoretical and experimental studies in the project, which is currently subdivided into four subprojects (SP): SP1 Three-Dimensional (3-D) Probabilistic Model of Deformable Cell Rolling and Adhesion, SP2 MPI Parallel Algorithm for Deformable Cell Motion and Adhesion; SP3 Monocyte and SP4 Platelet Interactions with Arterial Endothelium in Vitro.

Since the above-mentioned 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.

Preliminary results:

- In SP1, the Monte Carlo algorithm for probabilistic single bond kinetics has been

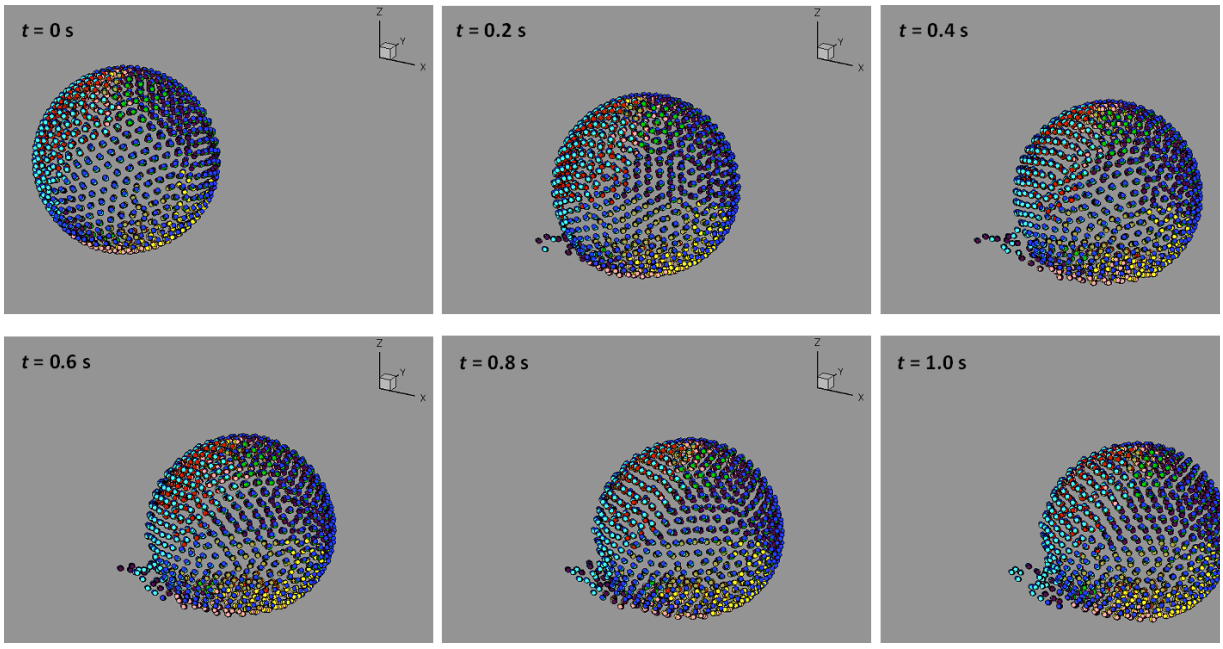

Figure 1. Changes in the spatial distribution of PSGL-1 (ligand for surface-bound P-selectin) expressed on microvilli of a rolling human monocyte, according to numerical simulation. The computational algorithm used in the simulation is the viscoelastic Volume-of-Fluid algorithm for two-phase flow combined with a Monte Carlo algorithm for stochastic receptor-ligand binding. Rolling of the cell on the P-selectin-coated lower plate of the microchannel (height = 15 μm) is mediated by P-selectin/PSGL-1 binding kinetics and the hydrodynamic force exerted on the cell by shear flow (wall shear stress = 0.5 dyn/cm^2). The cell has 729 quasi-uniformly distributed microvilli (not shown). Eight out of 25 PSGL-1 molecules present on the tip of each microvillus are marked by circles with different color fills.

implemented into the existing computational model of deformable cell rolling and adhesion. This allowed us to track the dynamics of individual receptor and ligand molecules during cell-cell interactions (Fig. 1). It should be noted that our computational model is an incompressible CFD code written in Fortran with OpenMP directives. The code finds the solution of the continuity and Navier-Stokes equations in three dimensions and takes into account viscoelasticity of the cell through the Giesekus model. Recent changes made in this code also include: 1) the Kelvin-Voigt model for viscoelasticity of microvilli (surface projections of the cell; previously we had elastic microvilli); 2) the model for tether extraction from microvilli (microvillus tethers behave as a Newtonian material). Currently, I am using the eight-processor node I purchased for the Tulane CCS to run the code. The following problems are being studied: 1) the effects of bulk deformability and microvillus properties on white blood cell rolling and adhesion in a microchannel and 2) the influence of tether extraction and catch/slip bond behavior on white blood cell rolling. The results of these studies were presented at the 2009 Fall Meeting of the Society of Rheology (SoR) and will be presented at the 2010 Fall Meeting of the Biomedical Engineering Society (BMES). This subproject involves collaboration with Drs. George Truskey (Duke U.) and Klaus Ley (La Jolla Institute for Allergy & Immunology, CA).

- In SP2, my graduate student Hongzhi Lan works on development of the MPI Parallel Algorithm for Deformable Cell Motion and Adhesion. His research was supported by 2009-2010 LONI Institute Graduate Fellowship. Currently, we have a working 2-D code for cell motion (adhesion is not yet implemented), which is used, together with the existing OpenMP 3-D model, to study separation of cells in a microchannel based on bulk deformability. We plan to apply for LONI allocation as soon as we implement the adhesion algorithm into the MPI code. External collaborators: Drs. Dino Di Carlo (UCLA) and Alex Alexeev (Georgia Tech).
- In SP3, my graduate student Chong Chen has conducted a series of experiments

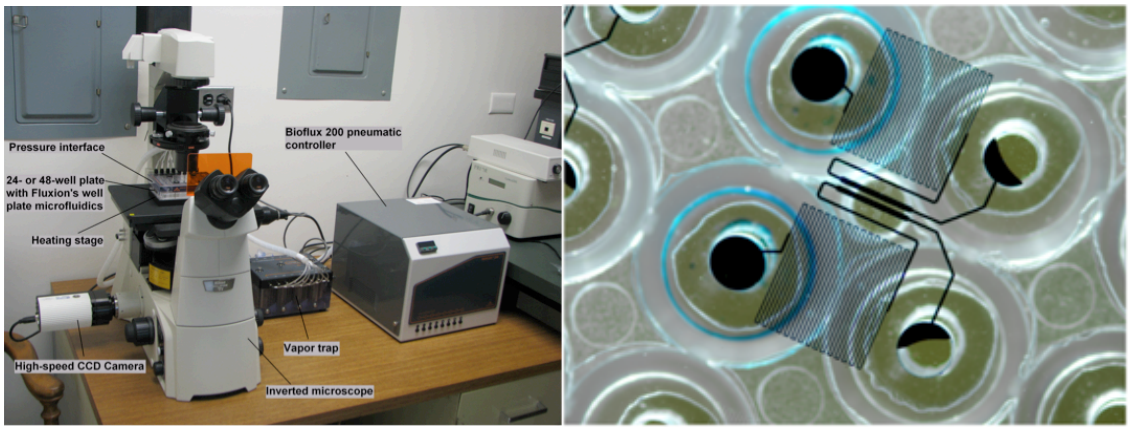

Figure 2. Photographs of the Bioflux 200 shear-flow system installed in Dr. Khismatullin's laboratory (LEFT) and bottom image of a Bioflux 200 48-well plate showing microchannels that connect inlet and outlet wells (RIGHT, from Fluxion Biosciences http://www.fluxionbio.com).

examining the effects of histamine, TNF-α, and OxLDL (inflammatory mediators) on THP-1 (monocytic cell line) interactions with HUVEC (endothelial cell line) in the Bioflux 200 microfluidic shear flow system (Fluxion Biosciences, CA; cf. Fig. 2). This

system was purchased and installed in my laboratory in summer 2009. It provides a better control over the rolling and adhesion processes than a conventional parallel-plate flow chamber. Our experimental data indicate that histamine may play an important role in development of an atherosclerotic plaque. The results of this research will be presented at the 2010 BMES Fall Meeting. In addition, Maria Belaidi (Tulane undergraduate student who worked in my laboratory in fall 2009 and spring 2010) conducted viability, proliferation, and static adhesion assays with THP-1 and HUVEC cultured at different temperatures. She determined the range of temperatures at which the cells remain viable (33 to 38.5˚C) and found that firm adhesion of THP-1 increases with temperature in this range, thus showing the direct relationship between white blood cell adhesion and increased body temperature in inflammation. This research involves collaboration with Dr. George Truskey (Duke U.).

- In SP4, Theodore Brown, a Tulane undergraduate student who conducts a senior design project in my laboratory, is working on development of a cell-free system to study platelet adhesion to endothelium. This cell-free system represents fluorescent carboxylate microspheres coated with Recombinant Human GPIb-α (platelet glycoprotein). We study how these microspheres interact with HUVEC under static and flow conditions. Our preliminary data indicate that HUVEC stimulation with histamine increases the number of firmly adherent microspheres under static conditions, which serves as additional evidence that histamine may be responsible for endothelial dysfunction occurring in atherosclerosis and thrombosis.

Project 2: Development of Novel Methods for Rheological Characterization of Biological Materials The overall goal of this collaborative project is to develop the techniques that will be able to measure rheological properties of blood, blood clots, white blood cells, and other biomaterials with better accuracy than the existing methods. Currently, this project has three subprojects: SP1 Acoustic Levitation Method for Noncontact Rheological Measurement of Biomaterials, SP2 Double Concentric Cylinder Rheometer with a Slotted Rotor for Characterization of Blood and Other Yield Stress Fluids, SP3 Multiple Particle-Tracking Microrheology for Measurement of White Blood Cell Viscoelasticity. My role in SP1 and SP2 are computational, i.e., my laboratory develops computational models that extract the values of material constants from the corresponding experimental data. In SP3, we conduct both theoretical and experimental studies.

Preliminary results:

- SP1 is a pending NSF grant application (see below), which has the following tasks: 1) development of a model for noncontact measurement of material constants through analytical studies and computational simulation; 2) development and validation of a noncontact acoustic levitation technique for the measurement of material properties of viscoelastic materials; and 3) application of the validated technique to biological materials, including blood clots and collagen gel. My laboratory will be responsible for Task 1 and participate in Tasks 2 and 3 of this grant application. All experiments will be performed in the laboratories of collaborating investigators (Drs. Holt and Zhang at Boston U.). Note that a blood clot consists of platelets and other blood cells embedded in a fibrin matrix. Currently, my undergraduate student Theodore Brown has written a Matlab code which determines the centroid and shape of a levitating thrombus from

experimental images. This information will be applied to the predictions of analytical and computational models to extract material constants.

- SP2 is a collaborative project with Dr. De Kee (Chemical & Biomolecular Engineering at Tulane; currently he is at NSF). Starting from August 2009, we co-advise the postdoctoral research of Dr. Weixiong Wang. In SP2, using the Fluent software package, Dr. Wang has conducted 2-D as well as 3-D CFD simulations to determine the differences in rheological measurements of yield stress fluids located between the slotted and non-slotted rotor designs in a double concentric cylinder rheometer. These simulations indicate that the rheometer equipped with a slotted rotor can measure the fluid properties with enhanced accuracy and less sensitivity to the wall slip velocity than a rheometer with a non-slotted rotor, which makes this design an excellent choice in rheological characterization of blood and other fluids with low value of yield stress. In his recent simulation, Dr. Wang found that this design is able to accurately measure rheological properties of a wide spectrum of test fluids, from Newtonian fluids to the fluids that significantly deviate from the Newtonian law. These results are included in two papers submitted to the Journal of Rheology (one of them is accepted for publication) and will be presented at the 2010 SoR Fall meeting. Based on this study, we plan to submit a NSF grant application in September.
- In SP3, my graduate student Yuan Teng measures rheological properties of biological solutions by multiple particle-tracking microrheology. This is the only method that can potentially measure the mechanical properties of white blood cells in vivo. In this method, thermal fluctuations in the coordinates of particles embedded in a test fluid are measured and the theory of Brownian motion (generalized Stokes-Einstein relation) is applied to the ensemble average mean squared displacement of the particles to determine the fluid material constants. Currently, we conduct validation studies, e.g., we confirmed that the method we use in the lab accurately determines viscosity of water and dextran solutions. Our next step is to study hydrogels and solutions of cytoskeletal proteins (e.g., actin). The ultimate goal is to develop the theory to predict the motion of particles embedded or present in the cytoplasm of white blood cells. It should be noted that the Stokes-Einstein theory does not work for living cells because of anomalous diffusion associated with active motion of cytoskeletal filaments.

Project 3: Numerical Study of Blood Flow in Cerebral Vessels with Aneurysm This is a collaborative project with Dr. Arthur Ulm in the Department of Neurosurgery at the LSU Health Sciences Center in New Orleans. Here, we are interested in development of computational models that will help understand why certain patients develop aneurysm in cerebral circulation and optimize the treatment (i.e., closure of the aneurysm with a special material) to prevent the further expansion of the aneurysm or formation of new aneurysms. **This 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**.

Preliminary results: Dr. Ulm's research group has isolated the giant intracranial aneurysm with surrounding vessels from a diseased patient. This aneurysm is the result of coalescence of two aneurysms, with the second one formed after the first surgical treatment. Dr. Weixiong Wang, a postdoctoral researcher working with me and Dr. De Kee, took images of the aneurysm and,

using the SolidWorks and Fluent software packages, we have developed a computational model for blood flow in the aneurysm and surrounding vessels (Fig. 3). Using this model, we found that the primary reason why certain patients develop intracranial aneurysm is a difference in vessel diameter between the left and right vertebral arteries, leading to increased static pressure in one of the sides in the basilar artery. We also found that blockage of the right vertebral artery during the first surgical treatment was responsible for formation of new aneurysm on the right side of the old aneurysm, eventually leading to patient death. The results of this study will be included in the paper that Dr. Ulm's group and my laboratory plan to submit to the Journal of Neurosurgery this August. This research is part of NIH grant proposal that I plan to submit this fall.

Project 4: Liver tumor ablation by combination of percutaneous ethanol injection and high-intensity focused ultrasound This project is a currently pending NIH R21 grant application. It involves collaboration with Dr. Matthew Myers (Food & Drug Administration), Dr. Charles Conway (a oncologic surgeon at Ochsner Medical Center), and Dr. Ronald Roy (Boston U.) The overall goal of the project is to develop a novel method for hepatocellular carcinoma treatment based on combination of chemical ablation via percutaneous ethanol

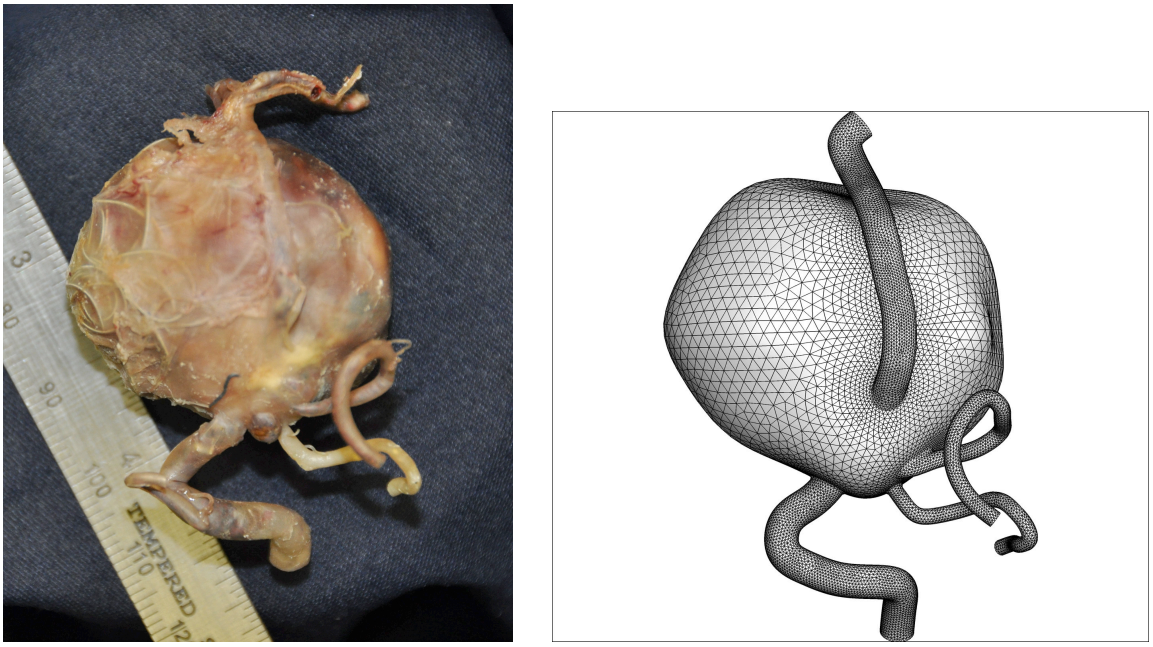

Figure 3. One of the photographs (top view) of a giant intracranial aneurysm formed in the vertebrobasilar system of a diseased patient (LEFT) and the geometry of the computational model constructed from aneurysm photographs (RIGHT). Three photographs were taken for the aneurysm from the top, front and right views. In each photograph, a ruler was put beside the aneurysm to provide a correct scale factor during the model construction. These images were imported into SolidWorks 2008 and selected as the top plane, front plane and right plane of the model, respectively. After alignment and scaling of the photographs, 3-D centerlines of the blood vessels and 2-D peripheries of the cross sections of the aneurysm were generated. Finally, blood vessels and the giant aneurysm were created in the model by the "sweep" and "loft" features in SolidWorks. Numerical simulation of blood flow in the constructed geometry was conducted using Fluent.

injection (PEI) and thermal ablation with high-intensity focused ultrasound (HIFU). The project involves computational studies of bubble cluster dynamics and ethanol diffusion in tissue during HIFU exposure (to be conducted in my laboratory), phantom studies and ex vivo studies with bovine liver (conducted at FDA), and in vitro studies with multicellular tumor spheroid cultures

(to be conducted in my laboratory using the cells isolated from tissue samples provided by Dr. Conway).

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 number of patients with advanced disease. Our project targets this group of patients.

Preliminary results:
My current effort in this project is development of the computational model for bubble cluster dynamics in tissue. Cavitation bubbles formed during ethanol injection and HIFU exposure play a critical role in tissue necrosis. My graduate student Chong Chen has received a FDA Summer Research Fellowship. From June 21 to August 21, she is working with Dr. Myers at FDA, where she learns experimental techniques that we will use in the project. The study she will conduct at FDA will provide preliminary data for the next submission of this NIH R21 grant application.

During the third year of the grant period, I have also continued internal collaboration with Drs. Ricardo Cortez and Lisa Fauci (Mathematics Department; our interests are to combine the immersed boundary and viscoelastic VOF algorithms to study numerically the effect of viscoelasticity on the motion of microorganisms) and Dr. Noshir Pesika (Chemical & Biomolecular Engineering). Our new project with Dr. Pesika is **to optimize the work of bent skimmers to rheological properties of oil spilled in the Gulf of Mexico.** In this project, which also involves collaboration with Dr. Alex Kolker from Louisiana Universities Marine Consortium, we will measure rheological properties of oil collected at different locations and depths in the Gulf of Mexico, develop a set of experimental and computational models of bent skimmers, and use these models to determine bent skimmer operating conditions and hydrophobic properties of its surface which leads to maximum efficiency of this device for a particular type of spilled oil.

Publications:

1. D.B. Khismatullin and G.A. Truskey, "The effect of cytoplasmic viscosity on leukocyte rolling on P-selectin explored by deterministic and stochastic simulations," *Biophys. J.* (to be submitted in July / August).
2. W. Wang, D. De Kee, and D. B. Khismatullin, "Comparison of vane rheometer and double concentric cylinder rheometer with a slotted rotor (DCCR/SR)" *J. Rheol.* (to be submitted in July).
3. J.C. Chrispell, R. Cortez, D.B. Khismatullin, and L.J. Fauci, "Shape oscillations of a droplet in an Oldroyd-B fluid," Phys. Fluids (to be submitted early July).
4. W. Wang, H. Zhu, D. De Kee, and D. B. Khismatullin, "Investigation of the reduction of wall slip effects for yield stress fluids in a double concentric cylinder rheometer with slotted rotor," *J. Rheol.* (in press).

5. D. B. Khismatullin, "The cytoskeleton and deformability of white blood cells" in Klaus Ley (Ed.), "Current Topics in Membrane. Vol. 64. Leukocyte adhesion", Birlington: Elsevier/Academic Press, pp. 47-111 (2009).

Presentations:

1. D. B. Khismatullin, "Computational modeling of leukocyte‐endothelial cell interactions in inflammation and atherosclerosis," 3rd CCT/LBRN Workshop on Computational Biology, March 27, 2010 — Baton Rouge, Louisiana.
2. D. B. Khismatullin, "Quantitative Biomechanical Models of Cellular Interactions," 2nd LONI Institute All-Hands Meeting, February 10, 2010 — Baton Rouge, Louisiana.
3. J. Chrispell, R. Cortez, D.B. Khismatullin, and L. Fauci, "The dynamics of immersed boundaries in viscoelastic fluids," 62nd Annual Meeting of the APS Division of Fluid Dynamics, November 22-24, 2009 — Minneapolis, Minnesota.
4. D.B. Khismatullin, C. Chen, G.A. Truskey, "Quantitative models of monocyte-endothelial cell interactions in atherosclerosis," 81st Annual Meeting of the Society of Rheology, October 18-22, 2009 — Madison, Wisconsin.
5. P. Stapor, W.L. Murfee, and D.B. Khismatullin, "Determination of Shear Stress Magnitudes Along Capillary Sprouts," 2009 BMES Annual Fall Meeting, October 7-10, 2009 — Pittsburgh, Pennsylvania.
6. J. Chrispell, R. Cortez, D.B. Khismatullin, and L. Fauci, "The dynamics of immersed boundaries in viscoelastic fluids," Mathematical Biosciences Institute (MBI) Workshop on Computational Challenges in Integrative Biological Modeling, October 5, 2009 — Columbus, Ohio.
7. D.B. Khismatullin and G.A. Truskey, "Modeling the mechanical behavior of white blood cells using a viscoelastic Volume-of-Fluid algorithm," 10th US National Congress on Computational Mechanics, July 16-19, 2009 — Columbus, Ohio.

External Funding:

1. National Science Foundation, Nano and Bio Mechanics Program. Title: *Collaborative Research: Noncontact Method for Rheological Characterization of Biological Materials* (pending). Role: Principal Investigator. Co-PI: R. Glynn Holt and Katherine Zhang (Boston U.).
2. National Institutes of Health, National Institute of Biomedical Imaging and Bioengineering (NIH-NIBIB). Type: R21. Title: *Liver tumor ablation by combination of percutaneous ethanol injection and high-intensity focused ultrasound* (pending; priority score: 52). Role: Principal Investigator. Collaborators: Matthew Myers (FDA), Charles Conway (Ochsner Medical Center), Ronald Roy (Boston U.).
3. National Institutes of Health, National Heart, Lung, and Blood Institute (NIH-NHLBI). Type: R21. Title: *Computational studies of leukocyte dynamics using micro-PIV in collagen microchannels* (priority score: 30). Role: Principal Investigator. Co-I: Sergey Shevkoplyas and Donald P. Gaver, III (Tulane U.).

Computational Free Energy Studies from Molecular Simulations

Principal Investigator:
David L. Mobley
Assistant Professor
Department of Chemistry
University of New Orleans

Research group:
Pavel Klimovich (graduate student), Anasuya Kolavennu (graduate student), Christopher Savoie (undergraduate student), Isabella Schmitt (undergraduate student), plus two incoming graduate students in Fall 2010. 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 Area, Specializations
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.

Project Description

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 fo 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, and are currently applying the approach to other protein binding sites including trypsin and HIV protease. 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 am beginning to develop collaborations with experimental groups at Louisiana State University (including Grover Waldrop and Fareed Qaddoura) and pharmaceutical companies. 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 currently supervise two graduate students and two undergraduate students, with additional graduate students joining the group in the Fall. Additionally, I handle graduate recruiting and selections for the Chemistry department, so there are a variety of outreach activities associated with that. I also recently co-organized a workshop on free energy calculations in drug discovery; this took place this Spring at Vertex Pharmaceuticals in Cambridge, MA.

Publications

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).

M. R. Shirts*, D. L. Mobley and S. P. Brown, "Free energy calculations in structure-based drug design", in "Structure Based Drug Design", Cambridge University Press (2010), edited by Kenneth M. Merz, Dagmar Ringe and Charles H. Reynolds. Invited chapter.

H. Kaur, S. Izenwasser, A. Verma, D. Wade, A. Housman, E. D. Stevens, D. L. Mobley, and M. L. Trudell*. "Synthesis and monoamine transporter affinity of 3α-Arylmethoxy-3β-arylnortropanes", Bioorg. Med. Chem. Lett. 10:6865-6868 (2009).

S. E. Boyce#, D. L. Mobley#, G. Rocklin, A. P. Graves, K. A. Dill, B. K. Shoichet. "Predicting ligand binding affinity with alchemical free energy methods in a polar model binding site", J. Mol. Biol. 394: 747-763 (2009).

D. L. Mobley* and K. A. Dill, "The binding of small-molecule ligands to proteins: 'What you see' is not always 'what you get'", Structure 17(4): 489-498 (2009).

D. L. Mobley*, C. I. Bayly, M. D. Cooper, and K. A. Dill, "Predictions of hydration free energies from all-atom molecular dynamics simulations", J. Phys. Chem. B 113: 4533-4537 (2009). Invited article, special issue on "Calculation of Aqueous Solvation Energies of Drug-Like Molecules: A Blind Challenge".

D. L. Mobley*, C. I. Bayly, M. D. Cooper, M. R. Shirts, and K. A. Dill. "Small molecule hydration free energies in explicit solvent: An extensive test of fixed-charge force fields", J. Chem. Theory Comput. 5: 350-358 (2009)

Presentations and Talks

"Insights and innovations in alchemical calculations of binding free energies", American Chemical Society Meeting, San Francisco, CA, March 21, 2010. Contributed talk.

"Predicting biomolecular binding interactions from thermodynamics," University of New Orleans Department of Physics, March 10, 2010. Invited talk.

"Predictive calculations of protein-ligand binding", Louisiana State University Department of Biological Sciences, Oct. 5, 2009. Invited talk.

"Insights from calculations of hydration and binding free energies", University of New Orleans Math Colloquium, Sept. 9, 2009. Invited talk.

"Alchemical predictions of free energies, from hydration to binding", American Chemical Society Meeting, Washington, D.C., Aug. 19, 2009. Contributed talk.

"Computational predictions of protein-ligand binding affinities", Hewlett Packard Outstanding Junior Faculty Award, American Chemical Society Meeting, Washington, D.C., Aug. 18, 2009. Invited talk.

"Explicit solvent calculations of transfer free energies", OpenEye SAMPL meeting, Montreal, Canada, June 18, 2009. Contributed talk.

"Lessons learned from predicting binding free energies in model binding sites" and "Quantitative predictions of protein-ligand binding affinities", American Chemical Society Meeting, Salt Lake City, UT, March 2009. Contributed talk.

"Predictive calculations of absolute binding free energies", American Chemical Society Meeting, August 2008, Philadelphia, PA. Invited talk.

External Funding (proposed, pending, awarded)

Received:
"Improving drug discovery and biomedical innovation using molecular simulations", Louisiana Board of Regents Research Enhancement Program, June 1, 2010 through May 30, 2011. $121,303. As PI.

"Advancing new computational methods for predicting protein-ligand binding", Louisiana Board of Regents Research Competitiveness Subprogram, June 1, 2010 through May 30, 2013. $132,375. As PI.

Pending:
"Improving alchemical methods for predicting protein-ligand binding", NIH R-15 grant, Feb. 25, 2010. $351,840. As PI.

"Leveraging next generation supercomputing to study complex emergent phenomena in novel materials", EPSCoR proposal, PI: Michael Khonsari. As co-investigator. Oct. 2009.

"High-Capacity Data Storage System for the University of New Orleans", Department of Defense, $269,760. As senior investigator. Sept. 2009.

White Papers for LONI Third Annual Report

Submitted by
Dr. Zhenyu Ouyang, LONI Assistant Professor
Department of Mechanical Engineering
Southern University and A&M College, Baton Rouge, LA
June, 2010

Part 1: Cover Page

Research group for Novel and Advanced Engineering Materials

Group Members:
Group PI: Dr. Zhenyu Ouyang, Assistant Professor
Graduate Students:
Mr. Jay Kumar
Mr. Morampudi Dheeraj
Mr. Raghvan Madawela
Mr. Gefu Ji (Co-advised)

Roles and Specializations:
Experimental, computational and theoretical studies on advanced engineering materials

Research Field:
Development and modeling of novel adhesively bonded joints; nonlinear fracture mechanics characterization of nano/micron fiber reinforced composite materials; shape memory alloy (SMA) metallic foam based sandwich structures for impact mitigation

Part 2: Project Description

Project 1 summary: Development and modeling of Novel Bonded Joints: Joints exist in almost all natural and man-made structures. Among all the joining/repairing methods, adhesive bonding is a focal technology due to its ease of assembling large and integrated structures with reduced weight, excellent corrosion resistance, simple implementation, more efficient aerodynamics and, often, reduced labor costs. There are two challenges for adhesive joints: The first is how to significantly and conveniently achieve high-strength, high-ductility, and high-reliability adhesive joints with improved microcracking threshold and leakage resistance for the applications in hazard environments and energy industries. The second is how to autonomously and efficiently repair the possible adhesive damages which are caused by fatigue or unexpected overloadings. In this project, we are developing a novel adhesive joint with self-prestressing, self-reinforcing and self-healing functions. It can be simply realized by filling regular adhesive in a thin layer of open-cell shape memory alloy (SMA) foam with negative Poisson's ratio (NPR). With the proposed idea, a novel joint with integrated features can be simply realized. In the

project, two tasks will be realized: 1) Experimental study on the effect of various physical parameters on the joint toughness and interfacial strength; and 2) computational modeling of the failure process.

Project 2 summary: Characterization of nano/micron short fiber reinforced materials: Many engineering materials, such as epoxy, ceramic, concrete as well as many refractory metals, play important role in modern industries. However, the above mentioned materials share a drawback that they are fundamentally brittle. To make these brittle materials tougher while still strong is always preferred for engineering applications. The addition of short fibers (nano-fiber or micro-fiber) in the brittle matrix is an effective approach. Without the short fibers, the short initiation and quick propagation of a few major cracks can cause brittle, sudden or even catastrophic failure of the materials and structures. Previous studies showed that the embedded short fibers can hinder the generation of major cracks by creating numerous micro-cracks. Meanwhile, the local deboning along the interfaces between matrix and fibers increase the fracture energy dissipation. As a result, the modeling work becomes more complicated. Originally, the homogenous and brittle materials can be conveniently and accurately modeled by the classical theory of fracture mechanics. Due to the inclusion of short fibers, somehow plastic behaviors can be achieved for the reinforced brittle materials. In order to accurately simulate the failure process, nonlinear fracture mechanics, specially, the cohesive zone model (CZM) may be desirable. The cohesive law is required as the fundamental input CZM. In this project, we are trying to characterize the cohesive laws for two materials: epoxy based syntactic foam and ultra-strength concrete, reinforced by with two relative new short fibers: basalt fibers and Cu based shape memory alloy (SMA).

Project 3 summary: Shape memory alloy (SMA) metallic foam based sandwich structures for impact mitigation: Sandwich structures based on high performance skins are currently finding widespread use in a number of aerospace, marine and automotive applications, where low weight, high strength and high stiffness are important design requirements. Many conventional sandwich structures are based on polymeric foams. In the past decade, metallic foam based sandwich structures are received rapidly increasing level of interest in investigating the potential offered by lightweight metallic foams for use in a range of high performance structural applications. Preliminary tests on closed-cell aluminum foams have shown that these materials offer improved soundproofing capability, low thermal conductivity characteristics. An important application of metallic foam based sandwich structure is for the impact mitigation due to its impressive impact energy absorbing capabilities. However, the permanent plastic deformation of ligaments conventional metallic foam when suffering impact hinders the multiple services for impact mitigation. In this project, we will achieve the sandwich structures with multiple services capability for impact mitigation by developing shape memory alloy (SMA) based metallic foam. There are two major advantages: First, the SMA ligaments themselves have significantly damping capability; second, the impact induced plastic deformation can be completely or largely removed by proper structural design due to the pseudo-plasticity of SMA.

The intellectual merit lies in its transformative approach to creating and advancing knowledge and technology in novel and advanced composite and functional materials & structures, and enhancing research infrastructure and competitiveness of the investigators in national R&D marketplace. It inherently consists of fundamental studies and applied research, which will attract researchers from various disciplines of applied mathematics, science and engineering. The merit also lies in the scientific research training to both graduate/undergraduate students,

particularly minority students, in the novel engineering materials and structures. The current research is also multidisciplinary, including mechanics, materials, chemistry and physics, based on a wide collaboration at the state of Louisiana, national and international level. For instant, several research proposals are based the collaboration between LSU and SU. A currently ongoing research project is based on the collaboration at the national level (NC and UT). In another funded project, a visiting scholar from China is involved; also see more details regarding collaboration in the section of research proposals.

The broader impact is substantial as it relates to almost all man-made infrastructure like aircraft, micro-chips, ship, auto, pipe, tank, platform, bridge, building, harbor, just name a few. The current research activities have impact on: 1) engineering education by creating on campus and inter-campus structural and materials courses; 2) underrepresented groups by involving and retaining minority students in the state-of-the-art research. So far, 4 graduate students and several undergraduate students have been involved in the current research projects; 3) industrial partners through workshop and technology transfer; 4) outreach to high school students and teachers by sponsoring Science & Engineering Fair Projects and hands-on demonstration of materials technology; and 5) economic development by providing value-added novel materials and structures to the civilian and military markets.

Enhance infrastructure for research and education: The PI reform the syllabus of his several classes at SU by including current research projects. He will present both basic science and applied technology to the students. This will strengthen not only the curriculum at SU but also enhance the research infrastructure by training the most active and creative element in research – human recourses for Louisiana. The College of Engineering at SU (the largest HBCU in Louisiana) has established a Master of Engineering program over years. Owing to the active and innovative research topics, three graduate students have enrolled this year. More research assistantship will become available to recruit and support graduate students. This will not only help the PI achieve national competitiveness, but also allow him to contribute immensely towards the engineering and science educational goals for minorities in Louisiana.

Part 3: Publications

Gefu Ji, **Zhenyu Ouyang** , Guoqiang Li, Samuel Ibekwe, and Su-Seng Pang, Effects of Adhesive Thickness on Global & Local Mode-I Interfacial Fracture of Bonded Joints, *International Journal of Solids and Structures* (In press).

Zhenyu Ouyang , Guoqiang Li, Samuel Ibekwe, Michael Stubblefield, and Su-Seng Pang, Crack Initiation Process of DCB Specimens Based on First-order Shear Deformation Theory, *Journal of Reinforced Plastics and Composites*, Vol. 29, No. 5,pp. 651-663 (2010).

Zhenyu Ouyang and Baolin Wan, An Analytical Model of FRP-Concrete Bond Deterioration in Moist Environment, *Advances in Structural Engineering*, Vol. 12, Number 6/December, pp. 761-769, 2009.

Gefu Ji, **Zhenyu Ouyang** and Guoqiang Li, Effects of Adhesive Thickness on Mode-II Interfacial Fracture Behaviors of Bonded Steel Joints, *International Journal of Solids and Structures* (under review).
Gefu Ji, **Zhenyu Ouyang**, and Guoqiang Li, Effects of Bondline Thickness on Mode-I Nonlinear Interfacial Fracture of Laminated Composites: An Experimental Study, *Composites Science and Technology* (Under review).

Zhenyu Ouyang, Gefu Ji and Guoqiang Li, On Approximately Realizing and Characterizing Pure Mode-I Interface Fracture between Bonded Dissimilar Materials, *ASME Journal of Applied Mechanics* (Under review).

Gefu Ji, **Zhenyu Ouyang** and Guoqiang Li, Dwayne Jerro and Su-Seng Pang, 2010, Effect of Bondline Thickness on Interfacial Fracture of Laminated Composite Materials, *ASME 2010 Pressure Vessels & Piping Conference*, July 18-22, 2010, Bellevue, Washington (in press).

Zhenyu Ouyang, Wei Xu, Gefu Ji, and Guoqiang Li, Dwayne Jerro and Su-Seng Pang, 2010, Nonlinear Model of Torsional Fracture in Adhesive Pipe Joints, *ASME 2010 Pressure Vessels & Piping Conference*, July 18-22, 2010, Bellevue, Washington (in press).

Gefu Ji, **Zhenyu Ouyang**, Guoqiang Li and Samuel Ibekwe, Effect of Adhesive Thickness on Interfacial Fracture of Bonded Steel Joints, *ASME 2010 Pressure Vessels & Piping Conference*, July 18-22, 2010, Bellevue, Washington (in press).

Zhenyu Ouyang, Gefu Ji, Guoqiang Li and Samuel Ibekwe, A New Idea of Pure Mode-I Fracture Test of Bonded Bi-Materials, *ASME 2010 Pressure Vessels & Piping Conference*, July 18-22, 2010, Bellevue, Washington (in press).

Zhenyu Ouyang, Gefu, Ji and Li, G., Simple Method for Characterizing Pure Mode I Interface Fracture Cohesive Law of Hybrid Joint Bonded with Dissimilar Adherends, *Society of Plastic Engineering-ANTEC 2010 Conference*, Orlando, FL, May, 2010.

Paper in Preparation:

Zhenyu Ouyang, Jay Perneedi, Guoqiang Li and Gefu Ji, Experimental characterization fracture behavior of glass microballoon filled lightweight reactive powder concrete, *Concrete and Cement Research* (to be submitted).

Zhenyu Ouyang, Vijay Morampudi, Guoqiang Li and Gefu Ji, Experimental and numerical study on the cohesive fracture behavior of SMA fiber reinforced syntactic foam, to be submitted to *Journal of Composite Materials*, (to be submitted).

Part 4: External Funding

Proposals Submitted as PI/Co-PI (in pending)

Smart Joint Bonded by Adhesive with Negative Poisson's Ratio and Shape Memory Capability, 09/01/2010-08/31/2013, $317,943 for three years, National Science Foundation, **PI: Dr. Zhenyu Ouyang**, co-PI: Dr. Guoqiang Li.

Multi-scale Simulation and Visualization for Refractory Materials Design, 09/01/2010-08/31/2013, $200,000 for three years, Department of Energy, PI: Patrick F. Mensah, co-PI, **Dr. Zhenyu Ouyang** and Dr. Amitava Jana.

Negative Poisson's Ratio and SMA Based Metallic Foam Reinforced Adhesive Layer in Bonded Joints for Aerospace Structures, LaSPACE Research Enhancement Awards Program, **PI: Dr. Zhenyu Ouyang**, co-PI: Dr. Guoqiang Li.

Proposals Submitted as PI/Co-PI (not funded)

Experimental Study and Numerical Simulation of Advanced Hybrid Joints Bonded with Shape Memory Alloy (SMA) and Shape Memory Polymer (SMP), 06/01/2010-05/31/2013, $118,751 for three years, Board Regent of Louisiana, **PI: Dr. Zhenyu Ouyang**, co-PI: Dr. Guoqiang Li.

Collaborative Research: Nonlinear Cohesive Fracture of Self-prestressing and Self-healing Adhesive Composite Joints with SMA Z-pins, 06/01/2010-05/31/2013, $177,978 for three years, National Science Foundation, **PI: Dr. Zhenyu Ouyang**, co-PI: Dr. Guoqiang Li.

Proposals to be submitted as PI/Co-PI

Fe-SMA based metallic foam embedded sandwich structures for impact mitigation, to be submitted to DEPARTMENT OF DEFENSE (DoD) at Aug. 2010, **PI: Dr. Zhenyu Ouyang**, co-PIs: Dr. Guoqiang Li and Dr. Samuel, Ibekwe.

Ongoing funded project as PI/Co-PI

"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), Guoqiang Li (PI) and **Zhenyu Ouyang** (Co-PI), $135,000 (**IDEA/TRB**) and $29,000 (LTRC matching); (3/1/2009–09/31/2010); Contract/Grant Number: Project 20-30, IDEA 142 (One visiting scholar from China is partially supported by this project).

"An Integrated Topology and Multi-Scale Optimization of Protective Structures" funded by Army Research Office, (Collaborated with North Carolina A&T State University and University of Utah); Sub-contract PI: G. Li, Co-PI: **Zhenyu Ouyang**, 07/01/09-06/30/12, $120,000.

Ongoing funded project as Key Personnel:

Smart Adhesively Bonded High-Performance Joint for Composite Structures" funded by NASA-BoR, PI, Pang Suseng, Co-PI: Guoqiang, Li, and Samuel, Ibekwe, $1,080,000, 10/01/2007-09/30/2010, grant number NASA/LEQSF (2007-10)-Phase3-01.

Population dynamics and connectivity of Blue Crabs

Investigator:
Caz Taylor, Assistant Professor, Ecology and Evolutionary Biology, Tulane University

Group Members
Erin Grey, Postdoctoral researcher, Ecology and Evolutionary Biology, Tulane University
Hideki Fujioka. LI Computational scientist, Tulane
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), Physics major, Tulane, computer modeling
Other Undergraduate field assistants :Nick Brasier, Shae Crain, Kyle Coblentz, Susan Chaisson

Project Description

***Summary*:** 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 and 2009 (~1 TB). Hideki rewrote the model in C++ and it is now running on a Mac Pro in my lab. Hideki is working 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. I have a computational undergraduate student intern, Michael Bartlein (physics major at Tulane), funded by the Center for Computational Science (CCS) in my lab this summer. Michael is working on the model and conducting research by simulating different scenarios of larval dispersal.
Field work to gather data with which to validate the model is ongoing. We have 9 people (4 Tulane undergraduates) and 5 other temporary staff collecting megalopal stage crabs in sites along the coast from Appalachicola, FL to Galveston, TX. We are also conducting plankton tows to sample larval stages of crabs. So far, we have conducted two tows taking samples from an oil-affected area and an unaffected area in Louisiana. Data from all this field is still being processed.

Presentations/Talks

- *Population dynamics of Blue crabs*. Taylor. LONI Institute all hands meeting Jan 2010
- *Connectivity of Blue crabs.* Taylor, Grey, Nero, and Ko. LBRN Workshop on Computational Biology March 2010 (invited)
- *Ecology of Estuaries on the Pacific and Gulf Coasts:* Taylor Louisiana Universities Marine Consortium (LUMCON) Feb 2010

External Funding

Awarded

- NSF 6/1/10-5/31/11. RAPID Deepwater Horizon oil spill: Impacts on Blue Crab population dynamics and connectivity. $200k
- LA SeaGrant. 5/1/10 – 12/31/10. Deepwater Horizon Oil Spill Effects on Blue Crab Recruitment $10k
- USGS 9/1/2009 – Aug 31 2010: Long-Term Estuary Assessment Group (LEAG) $23k

LONI Institute Whitepaper for the LONI Institute Third Annual Report

Principal Investigator:
Christopher M. Taylor
Assistant Professor
Department of Computer Science
University of New Orleans

Group Members:
Joseph Coco
University of New Orleans, Masters Student
Specialization: Prediction of Viral Integration Sites

A. Murat Eren
University of New Orleans, PhD Student
Specialization: Analysis of Microbial Diversity

Mohamad Qayoom
University of New Orleans, PhD Student
Specialization: Sequence Mapping and Databasing

Qi Zhang
University of New Orleans, PhD Student
Specialization: Analysis of RNA Sequencing Data

Project Description

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:

- Computational Prediction of Viral Integration Sites
  - Classification of sites using machine learning algorithms
  - Prediction of integration sites in various cell lines
- Analysis and Visualization of Human Microbiome Data
  - Classification of diverse constituents present in samples
  - Visualization of bacterial community composition
- 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 exon usage patterns in gene expression data
    - Finding effects of various microRNAs on gene expression

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 ongoing collaborations involves researchers at Tulane Health Sciences Center and Xavier University. This work is 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 beginning to look 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 is under development.

Another collaboration that is beginning this Summer involves a different researcher at Xavier University. Joseph Coco is working on a model for viral integration sites based on genetic and epigenetic features of various cell lines. With the adoption of high-throughput sequencing and its increasing availability to researchers, a large pool of mapped viral integration sites in various cell lines and for various viruses has become available. Joseph will use this data to train his model using machine-learning methods in order to predict viral integration sites in cell lines that have not yet been mapped. Our collaborator at Xavier University has a system set up to map integration sites in a given cell line that will be used in tandem with Joseph's predictions to validate our method.

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 affects 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.

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. In Microarray Analysis of the Physical Genome. *Methods in Molecular Biology*. 2009;556:191-203. ISBN: 978-1-60327-191-2, Humana Press.

Refereed Journal Articles:

- Guorong Xu, Claire Fewell, Christopher Taylor, Nan Deng, Dale Hedges, Xia Wang, Kun Zhang, Haitao Zhang, Qinyan Yin, Jennifer Cameron, Michelle Lacey, Zhen Lin, Dongxiao Zhu and Erik K Flemington. Transcriptome and targetome analysis in miR-155 expressing cells using RNA-seq. *RNA*. [In Press].
- 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.

Refereed Conference Papers:

- Mohamad Qayoom, Qi Zhang, and Christopher M. Taylor. F-Statistics Algorithm for Gene Clustering Evaluation. *First ACM International Conference on Bioinformatics and Computational Biology*, Niagara Falls Conference Center, Niagara Falls, NY, August 2010.
- Anindya Dutta, Neerja Karnani, Ankit Malhotra, Gabriel Robins and Christopher M. Taylor. Extraction of Human DNA Replication Timing Patterns from Discrete Microarray Data. *Third IAPR International Conference on Pattern Recognition in Bioinformatics*, Novotel St Kilda, Melbourne Austrailia, October 2008.

Presentations

Invited Talks:

- 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.*
- Christopher M. Taylor. Extraction of Human DNA Replication Timing Patterns from Discrete Microarray Data. *LONI All-Hands Meeting.* Baton Rouge, LA, October 2008.

Posters:

- Christopher Taylor, Neerja Karnani, and Anindya Dutta. Analyzing DNA Replication Timing in the Human Genome. *Experimental Biology.* Ernest N. Morial Convention Center, New Orleans, LA, April 2009.

Funding

Received

- PI: Christopher M. Taylor. Title: *Graduate Student Services Agreement* (A. Murat Eren). Source: Research Institute for Children. Amount: $15,142. Approved: May 2010. Funding Period: April 1, 2010 to December 18, 2010.
- PI: Christopher M. Taylor. Title: *Graduate Student Services Agreement* (Joseph Coco). Source: Research Institute for Children. Amount: $4,500. Approved: May 2010. Funding Period: May 17, 2010 to August 14, 2010.
- 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 Buyout Professional Service Agreement*. Source: Research Institute for Children. Amount: $13,530. Approved: January 2010. Funding Period: January 4, 2010 to May 15, 2010.
- PI: Christopher M. Taylor. Title: *Graduate Student Services Agreement* (Qi Zhang). Source: Research Institute for Children. Amount: $16,726. Approved: July 2009. Funding Period: August 16, 2009 to August 14, 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 31, 2010.
- PI: Christopher M. Taylor. Title: *Summer Salary Professional Service Agreement.* Source: Research Institute for Children. Amount: $36,080. Approved: March 2009. Funding Period: May 17, 2009 to August 15, 2009.

Pending

- PI: Christopher M. Taylor. Title: Computational Prediction of Viral Integration Sites. Source: Department of Defense. Amount: $49,495. Date Submitted: May 28, 2010. Funding Period: August 16, 2010 to August 15, 2011.
- PI: Jay K. Kolls, PI: Nikos Krypides, PI: David Welsh, Co-I: Bennett deBoisblanc, Co-I: Zhide Fang, Co-I: Xiaogeng Feng, Co-I: Michael J. Ferris, Co-I: Kyle Happel, Co-I: Natalia Ivanova, Co-I: Leann Myers, Co-I: Doan Nguyen, Co-I: Amrita Pati, Co-I: Judd Shellito, Co-I: Christopher M. Taylor. Title: *Respiratory Microbiota and Mucosal Immunity*. Source: National Institutes of Health. Amount: $5,256,604. Date Submitted: March 15, 2010. Funding Period September 30, 2010 to September 29, 2013.
- PI: Christopher M. Taylor. Title: *Mapping algorithms for high-throughput sequencing and discovery of exon junctions.* Source: Louisiana Board of Regents RCS. Amount: $111,296. Date Submitted: November 4, 2009. Funding Period: June 1, 2010 to June 30, 2013.

LONI 3rd Year Annual Report
Submitted by
Rachel Vincent-Finley, Ph.D.
LI Faculty, Assistant Professor of Computer Science
Southern University and A & M College

Project 1: Analysis of Molecular Dynamics Simulations

The approach to long time molecular dynamics investigated in Project 1 centers on a reduced basis approach using principal component analysis. As in the work of Amadei, *et al.* [1], the goal here is to identify the "essential" subspace, the subspace in which functionally relevant atomic motion occurs. Given a molecule containing n atoms one can represent the molecule in a $3n$ dimensional conformation space. A reduced basis of dimension k is obtained by performing principal component analysis on a collection of molecular conformations. In this work these conformations are output obtained from a molecular dynamics simulation. [9] The new coordinate system, the reduced representation, does not track individual atomic positions but the molecule or system as a whole with respect to independent degrees of freedom. Previous work has demonstrated that typical values of k are significantly smaller in magnitude than $3n$. For example, Romo reported that 70% of the side-chain activity of myoglobin is described with $k = 20$ ($3n = 459$). [7] Thus a reasonable k dimensional representation constitutes a viable reduction of the space of atomic motion.

After determining a reduced basis, equations of motion are defined to track molecular motion with respect to the defined reduced basis. In experiments with lysozyme, Amadei, *et al*. [1] conjectured that the defined reduced basis remains valid over several hundred picoseconds. However, careful consideration must be taken in choosing how many steps are appropriate with respect to the reduced basis since the number of steps will likely be dependent on the molecule or system in question. [3] An updating scheme will be implemented in this work to incorporate new information into the reduced basis.

Project 1 will investigate error bounds associated with approximating an energy function of a particular molecule with respect to a reduced representation. Further, Project 1 will explore how such functions can be generalized to represent a class of molecules. Once viable approximations of the dynamic activity of a system have been established general items of interest include implementing an updating scheme with respect to a reduced basis and investigating minimum criterion for implementing said updating scheme. These investigations seek to determine how well dynamic activity of a reduced representation can sample the conformational space of a system and to identify error bounds for a range of systems.

We expect that in the reduced space, longer time steps can be taken since the fast modes have been "filtered out". However, it has been reported that simply increasing the length of the time steps in the integration algorithms can lead to strained structures. [2] One approach to control this is periodic equilibration with respect to the reduced basis. Further investigation of methods to efficiently propagate dynamics in the reduced basis is a basic goal of this work.

Project 2: Molecular dynamics simulation of multilayer (SiO_2/Ta_2O_5) coatings

Collaborator: Stephen C. McGuire, Ph.D., Professor, Department of Physics,
Southern University and A&M College (SUBR)
LIGO[1] Scientific Collaboration (LSC) Principal Investigator

Project 2, is a new collaboration with the Southern University LIGO (Laser Interferometer Gravitational Wave Observatory) Research Group. The primary goal of Project 2 is to develop a predictive means for gaining insights into the microscopic mechanisms that lead to mechanical loss in LIGO optical coatings. In particular, we seek to predict materials properties and performance by building effective computational models of the coating 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. In doing so we extend the capability of our existing program of materials characterization and based upon X-ray absorption spectroscopic (XAS) methods for determining chemical composition and microscopic structural studies of multilayered dielectric mirror coatings. [4] In addition, the XAS methods are being complemented by atomic force microscope (AFM) and X-ray diffraction (XRD) measurements.

We will perform molecular dynamics simulations of Ta_2O_5 and TiO_2 molecular mixtures within multilayered dielectric mirror coatings 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. [5] We will 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 and assist in addressing the mechanical loss in the coatings. The need for, and interest in, modeling capability of coatings within LIGO has been recently demonstrated and has applications within advanced versions of gravitational-wave interferometers.

Funded by the National Science Foundation, the Laser Interferometer Gravitational Wave Observatory (LIGO) is managed by the California Institute of Technology and the Massachusetts Institute of Technology with the goal "to detect and study gravitational waves of astrophysical origin." [6] The LIGO Scientific Collaboration (LSC) partners scientists from universities and institutions nationally and internationally in research toward this effort. [10] Southern University participates in the LSC under the direction of Dr. Stephen C. McGuire.

Abbreviated References

1. A. Amadei, A. B. M. Linssen, and H. J. C. Berendsen, "Essential dynamics of proteins," *Proteins: Structure, Function, and Genetics*, vol. 17, pp. 412-425, 1993.

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[1] LIGO – Laser Interferometer Gravitational Wave Observatory - *www.ligo.caltech.edu*

2. A. Amadei, A. B. M. Linssen, B. L. de Groot, D. M. F. van Aalten, and H. J. C. Berendsen, "An efficient method for sampling the essential subspace of proteins," *Journal of Biomolecular Structure and Dynamics*, vol. 13, no. 4, pp. 615-625, 1996.
3. M. A. Balsera, W. Wriggers, Y. Oono, and K. Schulten, "Principal Component Analysis and Long Time Protein Dynamics", *Journal of Physical Chemistry*, vol. 100, pp. 2567-2572, 1996.
4. E.E. Doomes and S.C. McGuire, "X-ray absorption spectroscopy of doped and undoped multilayer (SiO_2/Ta_2O_5) coatings on fused silica (SiO_2) substrates", *Nuclear Instruments and Methods in Physics Research A*, vol. 582, pp. 245-247, 2007.
5. G. M. Harry (for the LIGO Scientific Collaboration), "Advanced LIGO: the next generation of gravitational wave detectors", *Classical and Quantum Gravity*, vol. 27, 084006 (12pp), 2010.
6. LIGO Scientific Collaboration. "LIGO: the Laser Interferometer Gravitational-Wave Observatory," *Reports on Progress in Physics*, vol. 72**,** no. 7, 076901, 2009.
7. T. Romo, "Identification and Modeling of Protein Conformational Substates," Rice University, Houston, Ph.D. Dissertation 1998.
8. T. Romo, J. B. Clarage, D. C. Sorensen, and G. N. Phillips Jr., "Automatic identification of discrete substates in proteins: Singular value decomposition analysis of time-averaged crystallographic refinements," *Proteins*, vol. 22, pp. 311-321, 1995.
9. P. E. Smith and B. Montgomery Pettitt. Extended system program for molecular dynamics. Department of Chemistry, University of Houston*,* Board of Regents, 1991.
10. Website: LIGO Scientific Collaboration: www.ligo.org

Grant Proposals Awarded

1. Louisiana Board of Regents – EPSCoR RII
Title: "Computational Science Workshops for Louisiana Educators"
Collaborators: Berta E. Rodriguez-Milla (LSU); Kathryn Traxler (LSU)
Funds Requested: $ 29,726.00 Date Awarded: 04/26/2010
Workshop Dates: 07/19/2010 – 07/23/2010
Workshop Location: Louisiana State University, 338 Johnston Hall
https://www.cct.lsu.edu/LAeducators

Grant Proposals Pending

1. Thurgood Marshall College Fund – Department of Defense Air Force Office of Scientific Research
Title: "Molecular Simulation in a Reduced Basis – Implementation and Analysis"
Funds Requested: $ 10,000.00 Date Submitted: 03/20/2010

2. National Science Foundation – Cyberinfrastructure Training, Education, Advancement, and Mentoring for Our 21st Century Workforce
Title: "CI-TEAM Demonstration Project: Alliance for Improving Science and Technology (AfIST)"
Collaborators: Deanna M. Roquemore (SU); Joseph A Meyinsse (SU)
Funds Requested: $ 249,820.00 Date Submitted: 04/27/2010

3. National Science Foundation – Broadening Participation in Computing
Title: "Collaborative Research: BPC-DP: Computational Science Workshops for Louisiana Educators"

Collaborators: Berta E. Rodriguez-Milla (LSU); Deanna M. Roquemore (SU); Kathryn Traxler (LSU)
Funds Requested: $ 593,289.00 Date Submitted: 05/12/2010

Presentation – Outreach

1. "Ph.D. Career Paths and Possibilities", invited panelist, April 8, 2010, sponsored by the Mellon Mays Undergraduate Fellowship Program and the Office of Career Development, Bryn Mawr College, Bryn Mawr, PA.

Appendix B

LI Computational Scientists White Papers

Hideki Fujioka,
Computational Scientist, Tulane University

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

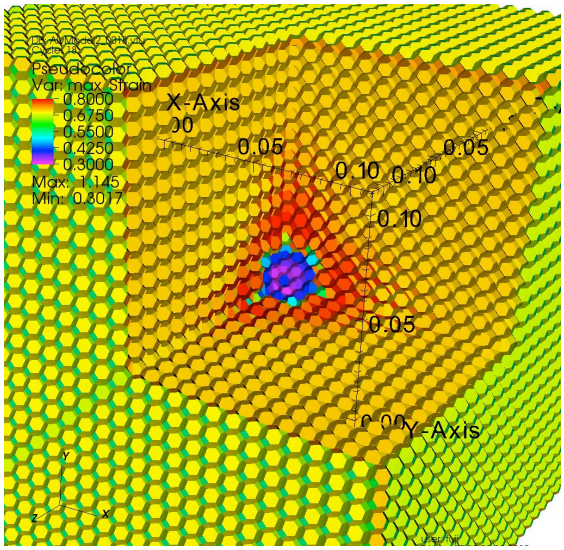
Project Description

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.

Pulmonary epithelial cells are exposed to mechanical stresses due to the stretch of the surrounding substrate and the motion of thin liquid film over them. There are a number of situations that these stresses becomes excessive, leading to cell damage or death. For example, local reduction of surfactant concentration results in nonuniform deformation of the parenchyma and the airways, and causes high membrane strain and high fluid stress due to high surface tension. Surface tension induces liquid flows, which may cause the lung's airways to close due to the formation of a liquid plug as a result of drainage of the liquid lining coating the airways or collapse of airway due to low pressure in the liquid. Once occluded either by a short plug or an extended collapsed region, the airway must be reopened to maintain ventilation to distal regions of the lung.

Though simplified models of airway closure and reopening phenomena in single airways have led to advances in our understanding of atelectrauma, the effect of the surrounding alveoli and the interdependence of airways on the these phenomena needs to be studied. In this study, we investigate the effect of parenchymal tethering on inflation/deflation mechanisms of atelectic regions of the lung. This will yield improved technologies for reducing the morbidity and mortality associated with respiratory distress syndrome and ventilator-induced lung injury.

We have constructed a 3D computational model of a truncated-octahedron alveolus based upon the work of Dale et al. (J.Biomech. 13, 1980). The displacement-based finite element method is used to analyze large deformation of the airway/alveolar system as a function of lumen, alveolar and pleural pressures as well as tissue constitutive relationships. A truncated-sctahedron with six square and eight hexagonal faces is used as a representation of the geometry in the model of the alveolus. Each face consists of supporting beams that have a non-linear stress-strain relationship to simulate the physical properties of elastin and collagen fiber bundles.



The figure shows an example of the results with the model. There are 25x25x25 alveoli with air-pressure of 10cmH2O. 15 alveoli with the surface tension of 65dyne/cm are place in the middle, simulating that surfactant deficient alveoli. The normal alveoli near the surfactant-deficient alveoli are stretched leading that their septal strain exceeds the normal range.

Presentation/talks
Biomedical Engineering Society, 2010 Annual Meeting.

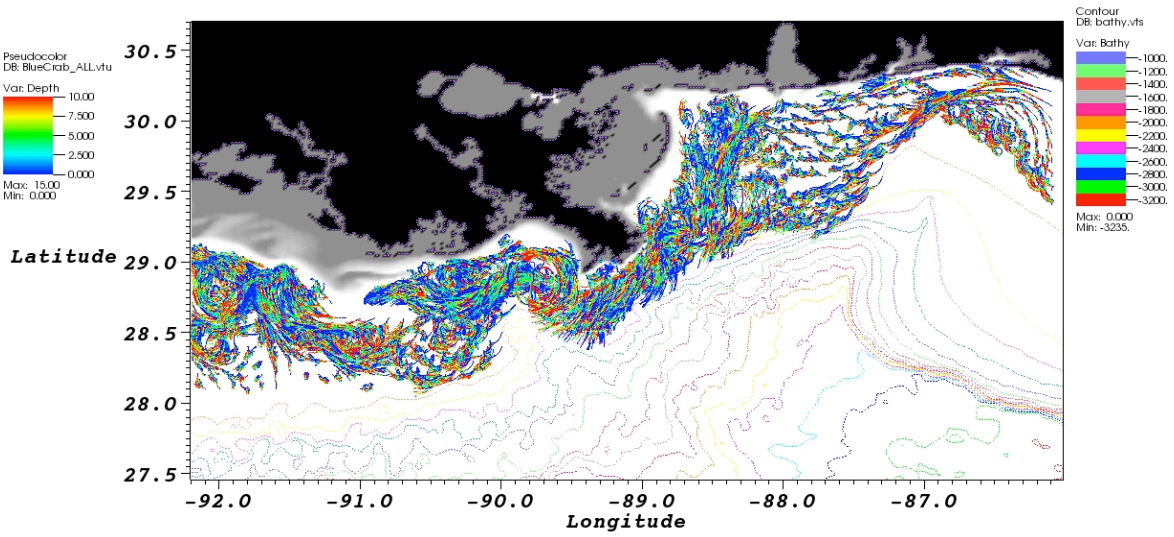
External Funding
N/A

Simulating Larval Dispersal in the Northern Gulf of Mexico
Caz Taylor, CCS & EEB, Tulane University
Richard Condrey, OCS & ACE, Louisiana State University
Woody Nero, NOAA National Marine Fisheries Service & Northern Gulf Institute
Erin Grey, EEB, Tulane University
Carey Gelpi, OCS & ACE, Louisiana State University

Project Description
Commercial fishing in the Gulf of Mexico generates more than $900 million per year, representing approximately 25% of fishing revenue in the U.S. Many of the organisms fished, such as crabs and shrimps, disperse as small larvae that drift in near-shore currents. Understanding this dispersal phase is crucial for developing predictive population models. Yet such understanding has proven difficult because near-shore currents in the Gulf are influenced heavily by winds and tides and because larvae often exhibit vertical swimming behaviors that can significantly alter their horizontal trajectories.

Recently, the Naval Research Lab has developed the Northern Gulf of Mexico Ocean Nowcast/Forecast System (NGOMNFS) which incorporates wind and tide data to resolve near-shore circulation patterns at a 1.9 km, hourly scale that is sufficient for tracking larvae. We are conducting larval dispersal simulations in the northern Gulf of Mexico by running a larval-behavior model through the archived NGOMNFS database (~1TB). The behavior model was written by Woody Nero at NOAA in Matlab and was parameterized for brown shrimp larvae. The Matlab version of the code is slow, taking 1 hour to simulate one night's release and dispersal of 500 larvae.

LI computational scientist, Hideki Fujioka has translated the Matlab code to C++ program to improve the computing time. Now it takes about 15 seconds to simulate one night's larvae tracking. The figure blow shows the blue crab pathway tracking for two days (4/1/2007~4/2/2007). It took about 30 sec to compute on 8-core Intel Xeon CPU Mac Pro.



Presentation/talks
N/A

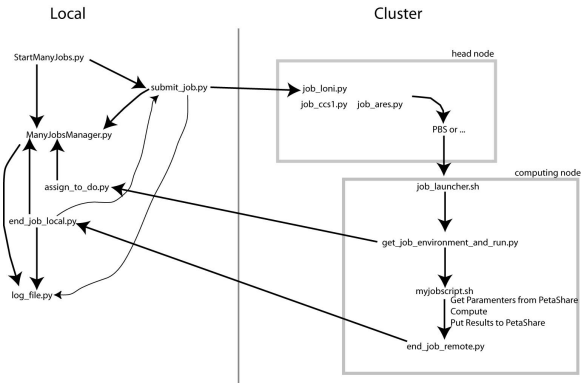
External Funding
N/A

Leveraging LONI Workflow Developments onto TERAGRID To Enable High Performance High Throughput Molecular Dynamics Simulations.
Thomas C. Bishop, CCS, Tulane University
Joohyun Kim and Nayong, CCT, LSU

Project Description
In an NIH funded study (R01GM076356) Bishop's goal is to investigate sequence dependent variations in nucleosome stability using molecular dynamics simulation techniques. Nucleosomes are the fundamental structural unit of chromatin and can be formed from any 146 basepair segment of DNA. In theory there are some 4146 possible sequences of nucleosomal DNA. In practice the ~12 million basepairs in the yeast genome position only about 60,000 nucleosomes (Jiang, et al., 2009). The degree of positioning ranges from highly positioned to nearly random positioning. Unfortunately, all available x-ray structures of the nucleosome have utilized nearly the same 146bp sequence of DNA (Luger, et al., 1997). We therefore have limited information on sequence induced structural variations in the nucleosome superhelix.

In order to submit jobs efficiently to several different clusters, LI CS Hideki Fujioka have developed a tool 'ManyJobs', which is written in python scripts. This tool submits jobs as much as possible to each cluster listed by the user. Once a job starts, the tool assigns a work to do. The followings are how the process goes: 1. Run “StartManyJobs.py” to start jobs; 2. “StartManyJobs.py” invokes “ManyJobsManajer.py” to get a list of clusters, name and the location of job-launching scripts, the number of jobs to submit for each; 3. “StartManyJobs.py”

invokes “submit_job.py”. “submit_job.py” runs the job-launching script on each cluster. The job-launching script submit a job into the queuing system; 4. “StartManyJobs.py” is finalized; 5. Waite until a job start; 6. Once a job starts running, “job_launcher.sh” invokes “get_job_environment_and_run.py” on the computing-node; 7. “get_job_environment_and_run.py” invokes “assign_to_do.py” on local machine; 8. “assign_to_do.py” invokes “ManyJobsManajer.py” to get a thing to do (if any) and send it back to “get_job_environment_and_run.py”; 9. “get_job_environment_and_run.py” sets environmental variables received from “assign_to_do.py” and invokes “myjobscript.sh”; 10. User should write “myjobscript.sh” as their needs. The script can use environmental variables set by “get_job_environment_and_run.py”; 11. Computing...; 12. When the computation is finished, “get_job_environment_and_run.py” invokes “end_job_remote.py”; 13. “end_job_remote.py” invokes “end_job_local.py” on local machine. “end_job_local.py” invokes “ManyJobsManajer.py” to report the job has finished; 14. “end_job_local.py” invokes “submit_job.py” to submit a new job onto the cluster which the job has finished. “submit_job.py” runs the job-launching script if there is still thing to do; 15. “job_launcher.sh” is finalized on the computing node; 16. goto 6.



Dr. Bishop was awarded a TERAGRID allocation (8,000,000SU) to conduct a larger study that is expect to produce some 40Tb of data. The project now aims at incorporating the 'ManyJobs' tool with PetaShare to manage the large data and many computations.

Presentation/talks
N/A

External Funding
N/A

Infrastructure for Accurate and Efficient Binding Affinity Calculations
David Mobley, Chemistry Department University of New Orleans
Steve Rick, Chemistry Department University of New Orleans
Shantenu Jha, Department of Computer Science Louisiana State University

Project Description
Accurate, reliable simulation-based tools for affinity predictions would transform the process of pharmaceutical drug discovery and enable new kinds of science. Recently, a tool called alchemical free energy calculations has shown considerable promise for predicting binding free energies from simulations. Several studies suggest these calculations could now be useful in practice in drug discovery and other applications, but for the difficulty of setting them up.

This project was to develop a pipeline to set up molecular dynamics simulations and associated alchemical free energy calculations, which would make it possible for these calculations to be more routine. This project involved three institutions in Louisiana State. The principal and co-investigators are David Mobley and Steve Rick at the University of New Orleans, and Shantenu Jha at Louisiana State University, and the LI Computational Scientist Hideki Fujioka at Tulane University, who helped to program computer codes.

The 'mmtools' package (https://simtk.org/home/mmtools) was modified to expand existing protein tools to allow user interventions such as specifying protonation states for selected residues (while assigning the rest automatically by 'mcce', http://134.74.90.158/). The interface of ligand building/protonation tools with protein/nucleic acid setup tools was added to allow easy setup of structures and parameter files for structures, together with ligands, including assigning all hydrogens and building in missing loops

Presentation/talks
N/A

External Funding
N/A

Dr. N. Raju Gottumukkala
Computational Scientist, University of Louisiana at Lafayette.

Group Members
Dr. Ramesh Kolluru, Director of NIMSAT Institute and CBIT
Dr. Mark Smith, Professor and Head of Department of Moody College of Business Administration
Dr. Baker Kearfott, Professor, Mathematics Department
Mr. Haochun Zhang, Student

Current Research
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, parallel algorithms, probabilistic modeling, and spatiotemporal optimization problems.

Inter University Collaborative Projects for 2010

Parallel Algorithms for Large Scale Data Clustering
Dr. Vijay Raghavan, Dr. Ryan Benton, Center for Advanced Computer Studies, UL Lafayette
Dr. Ramesh Kolluru, NIMSAT Institute, UL Lafayette
Dr. Box Leangsuksun, Department of Computer Science, Louisiana Tech University

The main goal of this LI project is to investigate optimal approaches to parallelize various clustering and association mining algorithms both on LONI and a prototype cloud cluster at the Center for Advanced Computing Center (CACS). The algorithms we develop help multiple interdisciplinary projects including Alzheimer's Disease Neuro Imaging Initiative (ADNI) datasets for characterizing and predicting dementia, spatiotemporal clustering of geospatial imagery and text mining of web data. The developed applications are expected to provide MPI/OpenMP/Hadoop implementations of data mining algorithms for LONI users upon validation. This project will also potentially advance the LONI infrastructure to support data parallelization using Map/Reduce frameworks such as Hadoop.

Parallel Optimization Algorithms for Disaster Management
Dr. Ramesh Kolluru, Dr. Mark Smith, NIMSAT Institute, UL Lafayette
Dr. Baker Kearfott, Department of Applied Mathematics, UL Lafayette

The NIMSAT Institute works on multiple research and development projects from multiple emergency management agencies including the Louisiana's Governors' Office of Homeland Security (GOHSEP), Department of Natural Resources (DNR) and Department of Homeland Security (DHS). These projects require developing algorithms and statistical models for enhancing disaster preparedness and response. The main goal of this project is to develop parallel optimization algorithms on LONI for enhancing various disaster management

applications such as evacuation models, site selection algorithms and infrastructure interdependency analysis.

iLevee: Intelligent Flood Protection Monitoring, Warning and Response System
Dr. Ramesh, Kolluru, NIMSAT Institute, University of Louisiana at Lafayette
Dr. Box Leangsuksun, Computer Science Department, Louisiana Tech University
Dr. Honggao Liu, Director of HPC, Louisiana State University, Baton Rouge, LA

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 under its responsibility. In this effort, DNR has funded a pilot implementation of this project through a collaborative effort of multiple organizations including Geocomp Corporation, PB Americas, Shannon & Wilson, James Lee Witt Associates, NIMSAT Institute at the University of Louisiana at Lafayette, SMARTEC and TIE Technologies.

The primary objective of this project is to develop and deploy an iLevee Central system that runs on LONI. iLevee Central is a highly-available iLevee Central system that will be deployed on LONI and parallelize various data processing and computation modules that will improve the response time of the iLevee Central.

Recent Publications

1. Gottumukkala, N. R., R. Nassar, C.B. Leangsuksun, M. Paun. “Reliability of a system of k nodes for high performance computing applications”. To appear in the March2010 issue of the The IEEE Transactions on Reliability.
2. 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.

Presentations

1. 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.
2. 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.
3. 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)

- "iLevee: intelligent Levee Monitoring System", funded by GeoComp Corporation/Louisiana Office of Coastal Protection and Restoration; $2,981,813 (contract under development).
- "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 (2008-2010).
- "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). Role: Co-PI.

Recent Outreach Activities:

- Mentoring the following students in LONI/ HPC Projects:
    a. Haochun Zhang, PhD Student, Department of Applied Mathematics, University of Louisiana at Lafayette
    b. Jessie Castille, PhD student, Department of Applied Mathematics, University of Louisiana at Lafayette
- Organized a LONI Workshop at University of Louisiana at Lafayette and gave a presentation on various hazard forecasting projects that use the TeraGrid.

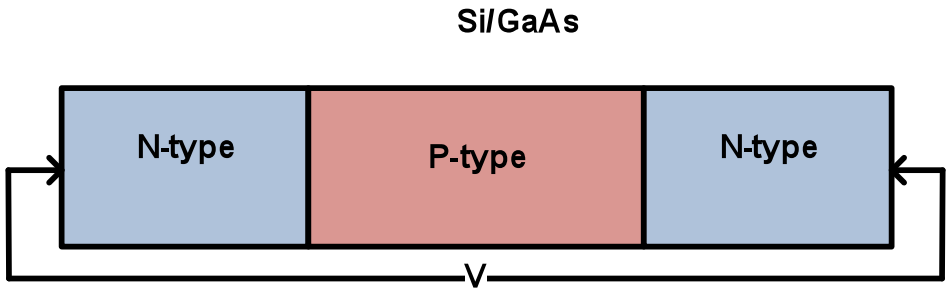
Mr. Abdul Khaliq
Computational Scientist, LA Tech.

RESERCH 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

Project 1
Surface Plasma Enhanced Solar Cells:

The electron generation in a three layered Si/GaAs device is analyzed with the state of the art semiconductor device simulator "MEDIC". The device is made of either Silicon or GaAs. The p-type Si/GaAs is sandwiched between two layers of n-type. A voltage is applied across the device.



The number of electrons increases in the p-type region with bias. The objective of this study is to determine a relation between the bias and the minimum number of electrons in the middle part. The population of electrons in the p-type region enhances with increasing bias. At a certain point the number of electrons is sufficient to cause a conduction. This is a turn on potential for this switch. This device works like a switch for surface palsmons. There is a coupling between two n-type regions when turn on potential is applied.

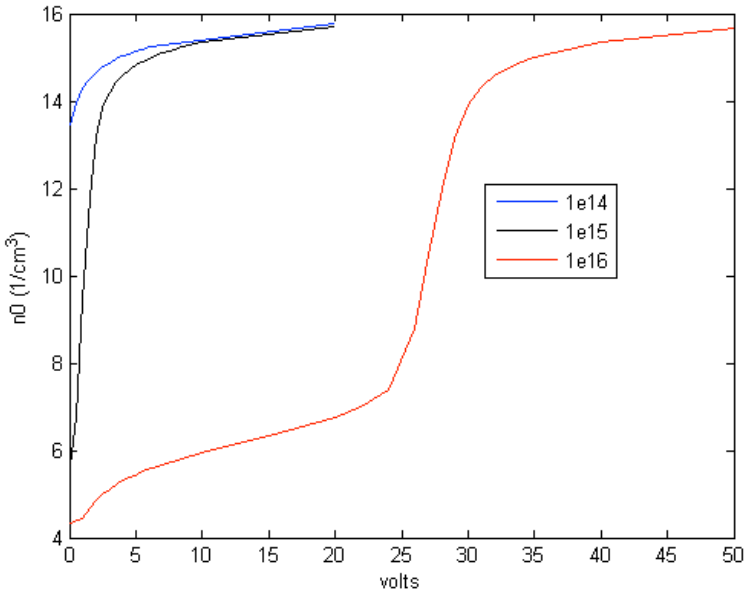


Figure 1: The bias versus electrons in the p-region in a Silicon

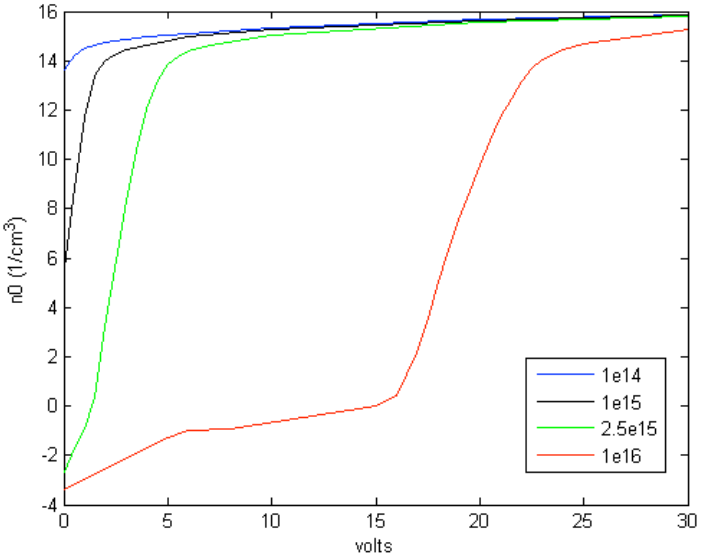


Figure 2: The bias versus electrons in the p-region in a GaAs

Project 2

Development of a full 3D Model for reaction-diffusion systems

A full 3D model of acetylcholine and acetylcholine receptor dynamics in the neuromuscular junction under conditions of inactivated enzyme has been developed. An improved Crank–Nicolson finite difference scheme is employed for solving the 3D model with Neumann boundary condition in cylindrical coordinates. In particular, a new, stable and accurate finite difference scheme is developed for the Neumann boundary condition. The simulation analysis agrees well with experimental measurements of end-plate current, and duplicates the open receptor results of earlier investigations. Sensitivity of the open receptor dynamics to the changes in the diffusion parameters has been studied. It presents the first simulation of asymmetric emission of acetylcholine in the synaptic cleft and an analysis of the subsequent effects on open receptor population as a function of time. Results show that the population of open receptors decreases as acetylcholine is emitted closer to the edge of the NMJ. Future investigations will focus in-depth study of anisotropic diffusion in the cleft, asymmetric distribution of vesicles in the pre-synaptic membrane, and completing the chemical reaction processes with the addition of acetylcholinesterase to the chemical kinetics of the NMJ.

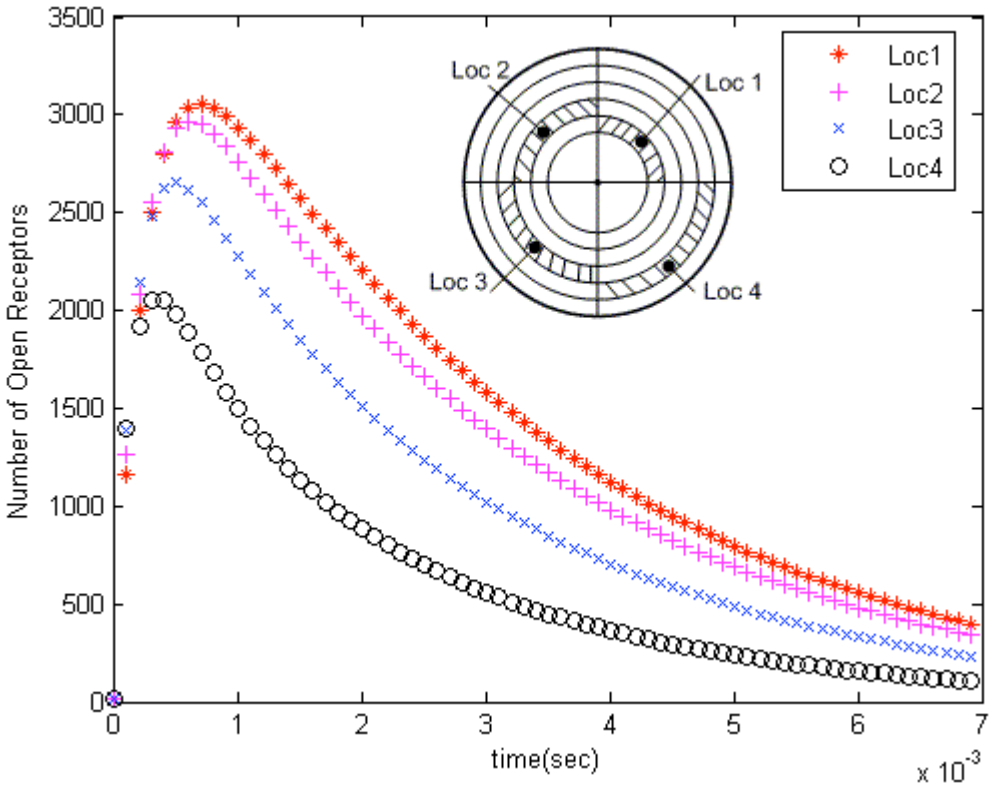


Figure 3: Sensitivity of open receptor dynamics to asymmetric Ach injection in different sectors

LONI Resources for Class Room Teaching

Collaborated with Dr. Dai to train students in using the LONI resources for Math 587 (ADVANCED SCIENTIFIC COMPUTING) to simulate:

a. Control volume method for solving 3D unsteady state Navier-Stokes equations and simulation techniques
b. FDTD and FDFD method for 3D electromagnetic simulation

Dr. Shizhong Yang
Computational Scientist, SUBR.

Group members:

Faculty: Dr. Ebrahim Khosravi; Dr. Shuju Bai; and Dr. Rachel Finley

Students: Graduate: Tianchuan Du; Kimberlee Lyles; Neelima Rama; Corey Baham; Goldie C. Jordan; Raghuvia Reddy Patlolla; Vani Panguluri; Kanukanti Rajendar; Annadasu Kiran Kumar; Kanetra Tillotson; Sai Ganesh Annamraju.

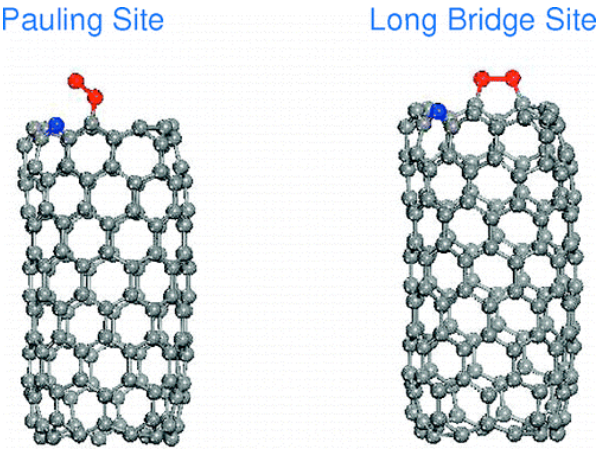
Undergraduate student: Theodore Newell; Laura Hurst

Research Fields: High Performance Computing; Computational Material; Computational Biology

Roles: Major Research Administrator

Project Description:

Computational Materials: (1). In this NASA supported highly reflective thermal barrier coating project, we performed *ab initio* electronic structure simulation on the 25% Ni doped ZrO_2 and found that the structure of 25% Ni doped at substitute site with a Zr vacancy is in a stable state. The reflectivity at different directions is evaluated by calculating the real and imaginary part of the dielectric constants. The result shows that the reflectivity of Ni doped ZrO2 crystal, with a Zr vacancy structure, varies from 59% to 80% at (001) ~ (111) directions respectively. In comparison, the reflectivity of pure ZrO2 is only 18% in the infrared wavelength range. The high reflectivity of 25% Ni doped ZrO2 structure, with a Zr vacancy, is caused by the unique doped crystal structure and the associated vacancy charge state in this configuration. (2). We also performed *ab initio* molecular dynamics simulation of 1:1 Ta doped YSZ system and found that the system has a very stable structure. (3) The simulation on nitrogen substitutionally doped short (10, 0) carbon nanotubes (CNTs) for dioxygen adsorption and reduction was performed. Our calculated results show that nitrogen prefers to stay at the open-edge of the short CNTs. Dioxygen O_2 can adsorb and partially reduce on the carbon−nitrogen complex site (Pauling site) and on carbon−carbon long bridge sites at the open-edge of the CNTs. The results of the spin polarization calculations show that the carbon atoms on the open-edge of the CNT can possess a magnetic moment of about 0.59 μB/atom, while those carbon atoms in the inner wall of the CNT do not have a magnetic moment. The doped nitrogen in the CNT does not have a magnetic moment. The chemisorption of dioxygen O_2 on the open-edge of the short CNT reduces the magnetic moments of the carbon atoms to nearly zero. Our published result is shown on the left right side of the graph.



The project is very successful and we generated 5 NASA/BoR/NSF related funding from this work. Most of publications are concentrated on this project. Supported by the funding, we made several travels to: (a) UCSD ICMPro workshop; (b) Q-Chem UC Berkeley workshop; (c) Laser Heating workshop at DOE-UC Berkeley Lab; (d) ICCS 2009 conference. We also set up close relation with NASA Glenn Research Center at Ohio. We invited Dr. Jeffrey at GRC come to LSU/SU making a talk and discussing our research finding on February 19. The extended NASA supported project and N doped CNT project were approved by LONI in the current fiscal year.

Computational Biochemistry: We first predicted the secondary structure of two membrane proteins gK and UL20. Our results are close to the predictions and experimental results available in literatures (one to two sequence secondary structure difference out of 200~300 amino acids). This laid the solid basis for our gK/membrane and UL20/membrane atomic modeling and MD simulations. Kimberle Lyles set up a model for the first segment of gK inside the membrane. The systems are very complex because the protein structures of gK and UL20 are unavailable. The modeling result was presented at the 84th LAS annual conference. Since part of our Molecular Dynamics work in this part was selected to the LBRN big proposal submitted to the NIH. Currently Kimberlee Lyles is finalize the NAMD simulation of gK/membrane and finish her Master thesis in this summer. The present LONI approved AA/8R-LOX docking using ICMPro is ongoing and we tested with a simple nitroapocynin/p47phox system. The NAMD simulation on the docked AA/8R-LOX simulation is ongoing.

Student research training: Training minority especially HBCU students is our important session in SU, which is the largest HBCU campus. We supported 10 students, all of them are minority students, in performing the state-of-the-art research. Students are trained in using our workstations, HPC machines at SU/LONI/TeraGrid. They also had close contact with LSU colleague student and faculty members. They joined LBRN/LONI conferences and several workshops, such as UCSD ICMPro workshop. We are very confident that our minority students got well prepared for the future higher level research and study.

We setup a dedicated HPC Lab for biology and material simulations in T. T. Allain Hall, Room 111B and 111D. A HP XW9400 Linux workstation, GraphStream Window X64 workstation, and several brand new PCs were purchased by our faculties' funding support and are currently fully functional for faculty and students performing research work. ICMPro, wxDragon, VASP, Wien2K, CHARMM, NAMD, Moldy etc. packages are purchased (or free downloaded and installed) at our machines. Currently there are 8 students working in our faculty funding projects. Four papers were published, several more are pipelined to be submitted.

Publications:

1. 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** 1102-1028 (2010).
2. 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** 3371-3375 (2010).
3. 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** 877-880 (2010).
4. Shizhong Yang, Shengmin Guo, Guang-Lin Zhao, and Ebrahim Khosravi, Highly infrared reflective nickel doped ZrO2 from first principles simulation, page 1~8, ICCS 2009, http://www.science.uva.nl/sites/iccs-meeting/iccs2009/PosterPapers/Poster-paper02.pdf .

Presentations:

1. APS March Meeting, S. Yang, E. Khosravi, and G.L.Zhao, Nitrogen doped carbon nanotubes for dioxygen reduction from ab initio simulations, Portland, Oregon, March 15-19, 2010.
2. 84th LAS Annual Conference: K. Lyles, S. Bai, E. Khosravi, and S. Yang, Modeling a gK protein fragment with a POPE Membrane, Alexandria, Louisiana, February 27, 2010.
3. MGCMM2010, G.L. Zhao, S. Yang, and E. Khosravi, Large-Scale First Principles Computations of Nitrogen Doped Carbon Nanotubes for Dioxygen Reduction, Baton Rouge, Louisiana, February 10-14, 2010.

External Fundings:

(1). 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: Ta_2O_5 Doped Zirconia: Simulation and Evaluation (PI: S. Yang)
Source of Support: Louisiana Board of Region (Pilot Fund)
Award Amount (or Annual Rate): $____10,000__
Period Covered:___1/01/2010-- 8/30/2010__

Location of Activity: SU-BR

Title: First Principles Simulation the Optical Property of Ta and Y 1:1 doped ZrO_2 (PI: S. Yang)
Source of Support: LaSPACE (CSG)
Award Amount (or Annual Rate): $____10,000__
Period Covered:__1/01/2010-- 12/31/2010__
Location of Activity: SU-BR

Title: NASA-LaSPACE Fellowship
Source of Support: LaSPACE (PI: S. Yang)
Award Amount (or Annual Rate): $____40,000__
Period Covered:__6/01/2010-- 5/31/2012__
Location of Activity: SU-BR, LSU

(2). Submitted/Pending:

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: 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): $__180,000_(SUBR)_
Period Covered:__10/01/2010-- 9/30/2013_
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

Dr. Zhiyu Zhao
Computational Scientist, UNO.

Group Members:

Austin Orgah (graduate assistant, Department of Computer Science, University of New Orleans)

Peiran Xu (summer undergraduate student worker, Department of Electrical Engineering, University of New Orleans)

Kristen Johnson (summer undergraduate student worker, Department of Computer Science, University of New Orleans)

Institutional Affiliation:

Department of Computer Science, College of Sciences, University of New Orleans

Roles and Specializations:

Please see Project Description

Research Fields:

Bioinformatics algorithms and applications; parallel and distributed algorithms and applications

Projects Description

1. A Parallel Protein Structure Alignment Tool and a Shared Feature Database for Structures in the Protein Data Bank

Role: PI

Collaborator: Dr. Christopher Summa, Department of Computer Science, University of New Orleans

Graduate Student: Austin Orgah

Description:

The research of proteomics has many biological applications. Proteomics research topics are usually related to protein sequences and structures. While both have close relationship with proteins' biological functions, structures reveal more evolutionary information than sequences do, since the structure of a protein changes more slowly in evolution than does its sequence. Also, researchers frequently find that proteins with low sequential similarity are structurally homogenous. Therefore it is particularly important to discover the structural similarity / dissimilarity among different proteins. The research of protein 3D structure similarity provides fundamental and very helpful tools for many biological research topics.

Result from protein structure determination techniques, the number of proteins discovered by biologists has increased dramatically over the last 30 years. The rapid growth of the Protein Data Bank (PDB) necessitates the development of efficient and accurate protein structure comparison and searching algorithms and automatic software tools.

We have developed a Self-Learning and Improving pairwise Protein Structure Alignment (SLIPSA) algorithm. SLIPSA is a feedback algorithm for protein structure alignment that uses a series of phases to improve the global alignment between two protein backbones. Based on a large set of proteins collected from various publications for diverse testing purposes, we have compared our algorithm with three other commonly used methods: CE, DALI and SSM. The

results show that in most cases our algorithm is more accurate than those well-known methods that have been tested.

The SLIPSA algorithm is implemented with MATLAB and we have developed a web portal based on it (see http://fpsa.cs.panam.edu/). Due to the large size of the PDB and high complexity of current protein structure alignment algorithms, an alignment can be very time-consuming and computation capability of machines greatly affects alignment performance in terms of both speed and accuracy. Since our current tool is just a proof-of-concept system written with MATLAB, there is a lot of space to improve its speed performance by (1) rewriting the code with C/C++, (2) taking advantage of parallel and distributed computation power of high performance computational resources, and (3) design an efficient protein database to store as much as possible offline information to reduce the execution time used by repetitively retrieving and calculating information from original protein data files.

We have migrated our MATLAB code onto the LONI and TeraGrid by rewriting all the code with serial C++, using OpenMP to implement a parallel version of the code, and deploying the code on Queen Bee. Austin, the graduate assistant, is developing a protein feature database for proteins in the PDB and we will deploy it on Queen Bee once it is completed. The database will hold protein features, both sequential and structural, for protein related research topics.

We have been awarded grant by the TeraGrid Pathways Fellowship Program to support Austin for fall 2009 to work on this project, which is now a part of the student's graduate thesis project. Drs. Summa and Zhao are jointly supervising the student.

2. Computational Infrastructure for Genome-wide Change Point Analysis at Basewise Resolution and Characterization of Transcriptome on the Isoform Level

Role: Co-PI

Collaborators: Drs Dongxiao Zhu (UNO), Kun Zhang (Xavier) and Erik Flemington (Tulane)

Undergraduate Student: Peiran Xu

Description:

(1) Computational Infrastructure for Genome-wide Change Point Analysis at Basewise Resolution

Our goal is to develop a computational infrastructure for performing genome-wide change point analysis with base-wise resolution. Our experimental system is the detection of miRNA targets on the genome scale. miRNA is a recently discovered gene regulation mechanism that down-regulates gene transcription and translation by Watson-Crick paring with target sites. More than 80% of human diseases have been shown to be intimately related to miRNAs. miRNA target prediction on the base-wise resolution has become a promising way to discover disease genes.

We propose to develop a computational infrastructure to run the change point analysis at basewise resolution for the human genome. The infrastructure is parallel computing in nature, since the problem size makes it infeasible on any single workstation.

(2) Computational Characterization of Transcriptome on the Isoform Level

Our goal is to develop a computational infrastructure for automatic characterization of transcriptomes on the splicing isoform level. Due to inherent limitations of hybridization based expression microarray technology, it only allows for the characterization of transcriptomes at the gene level. However, in the real biological system, the ultimate effectors on the transcription level are the splicing isoforms. One gene can be alternatively spliced into different isoforms of

transcripts in different tissues. Despite providing output on overall gene expression, isoform analysis using microarray data is computationally inaccessible.

The real challenge comes in the computational side in that the same iterative algorithm must be applied to a total of 22,000 genes annotated in human genome. The computational complexity of each gene is $O(M^2N)$, where M is typically 50 to a few hundreds, and theoretically N can be exponential to M. 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.

Tasks that have been accomplished or are ongoing include: (1) A C++ program has been developed to use the Schwarz Information Criteria (SIC) based method to detect change points; (2) Raw data (human chromosome 1, two samples, six lanes per sample) from Dr Zhu have been preprocessed before change point detection; (3) The program and data have been uploaded to Queen Bee and executed to detect all the change points in each gene; a gene annotation file has been downloaded from a public website and used to locate the start and end positions of each gene; (4) The result has been sent to Drs Zhu and Flemington for further analysis; (5) An undergraduate student worker is working under Drs Zhu's and Zhao's guidance on a parallel version of this change point analysis program; (6) *De novo* self-assembly tools have been installed on Queen Bee; (7) Simulated data with different short-read lengths (25, 36, 50, 75, 100) have been used to perform transcriptome assembly; (8) The assembly results are being validated using sequence mapping tools.

3. Improving Antibody Design by Structure Prediction, SCOP Classification and Protein - Protein Docking

Role: Co-PI

Collaborators: Drs Seth Pincus (LSU-HSC & RIC), Bin Fu (UTPA)

Undergraduate Student: Kristen Johnson

Description:

We propose to use a structure similarity search tool that we have developed in conjunction with existing structure prediction and protein - protein docking tools to improve the structural design of an antibody. We will be able to test experimentally the computational prediction of improved design by altering the amino acid sequence and determining whether the resulting antibody has the expected immunological characteristics. Antibodies can be used for molecular measurement and to treat diseases. The efficacy of antibodies is related to binding affinity. The software we propose to develop will allow computational prediction of higher affinity antibodies; such tools are of potential value to biotechnology and pharmaceutical companies.

The antibody, RAC18, we will be working with is a well-studied molecule, which binds to the plant toxin ricin, a material of biodefense concern. This antibody has been shown to be of protective efficacy in animal models, even when administered hours after the toxin. We now wish to improve the affinity of this antibody. The amino acid sequences of the heavy and light chain variable regions are known, as are the amino acids that the antibody contacts on the ricin molecule. Once computational predictions have been made regarding specific alterations to improve binding to ricin, we will use genetic engineering technologies to make that antibody and test it to determine if we have improved the affinity of binding to ricin and its protective efficacy in vivo.

All the software development work will be performed on a LONI cluster such as Queen Bee. These specific experiments may significantly improve the function of a clinically important antibody. By addressing this theoretically important issue in a well-characterized experimental system these studies may represent the initial steps in the production of more general tools for enhancing antibody and protein design. The successful prediction of protein improvements by a computational approach would be an important accomplishment in the field of bioinformatics.

Tasks that have been accomplished or are ongoing include: (1) An IgBLAST tool has been used to search for similar sequences with RAC18, the antibody that Dr Pincus' research group at RIC is interested in; (2) A structure search tool developed by Drs Fu and Zhao's group has been used to search for similar structures with RAC18; (3) Three antibody modeling tools have been used to predict the 3D structure of RAC18; a student worker at UNO (hired by RIC) is using these antibody modeling tools to predict the structures of proteins outputted from the above work; (4) Three antibody-antigen docking tools have been used to predict the docking orientation of some antibody models (either predicted or real, outputted from the above work) to the ricin toxin, the antigen of RAC18; The student worker will be using these tools to dock more structures (outputted from the above work) to the ricin; (5) A PyMOL add-in software tool is being developed to incorporate all the work into a uniform GUI, which also visualizes antibody/antigen/antibody-antigen complex structures and displays helpful information derived from them; (6) RAC18 related lab work is ongoing at RIC in order to get a thorough understanding about the production and functioning mechanism of RAC18.

Publications (07/01/09 - 06/30/10)

1. Zaixin Lu, Zhiyu Zhao and Bin Fu, "Efficient Protein Alignment for Protein Search", *BMC Bioinformatics* 2010, 11(Suppl 1)**:**S34, January 2010 (http://www.biomedcentral.com/1471-2105/11/S1/S34), and the Proceedings of the Eighth Asia Pacific Bioinformatics Conference (APBC 2010, India).
2. Bin Fu and Zhiyu Zhao, "Separating Sublinear Time Computations by Approximate Diameter", *Journal of Combinatorial Optimization*, 18(4): 393, November 2009.
3. Zaixin Lu, Zhiyu Zhao, Sergio Garcia, Krishnakumar Krishnaswamy, and Bin Fu, "Search Similar Protein Structures with Classification, Sequence and 3-D Alignments", *Journal of Bioinformatics and Computational Biology*, 7(5): 755 – 771, October 2009.
4. Huimin Chen and Zhiyu Zhao, "An Information Theoretic Viewpoint on Haplotype Reconstruction from SNP Fragments", the Proceedings of the 3rd International Conference on Bioinformatics and Biomedical Engineering (iCBBE 2009, China).

Presentations / Talks (07/01/09 - 06/30/10)

1. 12/07/09: "Improving Antibody Design by Structure Prediction, SCOP Classification and Protein - Protein Docking", Research and Education Building, Children's Hospital, New Orleans; a presentation to bioinformatics faculty at the University of New Orleans and the Research Institute for Children, Children's Hospital New Orleans.

2. 10/14/09: “Introduction to the Supercomputing Resources at LONI & TeraGrid”, Liberal Arts Building, UNO; An opening presentation for the undergraduate seminar in the Department of Computer Science in fall 2009.
3. 10/07/09: “Classification of Leukemia Patients via Micro-array Data Analysis”, CERM Building, UNO; A talk to Dr. Dongxiao Zhu’s research group with members from the departments of Computer Science and Electrical Engineering at UNO, the New Orleans Children Hospital, Tulane University, and Xaiver University.

External Funding (07/01/09 - 06/30/10)

1. NIH ARRA: Administrative Supplements Providing Summer Research Experiences for Students and Science Educators

Role: Co-PI

A project proposal titled “A new informatics paradigm for reconstructing signaling pathways in human disease” was submitted in summer 2010 and $200,294 total direct and indirect costs were proposed for the entire project period.

2. Research Institute for Children, Children’s Hospital New Orleans: summer research support

Role: PI

Kristen Johnson, the undergraduate student worker, has been hired by RIC to help collect research data for Dr. Zhao on the antibody structure improvement project mentioned above. She will be paid $1,000 per month, $3,000 in total during the period of May 17, 2010 – Aug 14, 2010.

Appendix C

LI Projects 2010-2011

Next Generation Parallel Codes for the Simulation of Correlated Materials

M. Jarrell, J. Moreno and J. (Ram) Ramanujam

The Project. Strongly correlated electronic materials, including spintronic and high-temperature superconducting materials, have many promising applications. The 2007 International Technology Roadmap for Semiconductors stresses that these systems can enable new devices by greatly enhancing their sensitivity to different applied fields. These materials also have promising applications in energy conversion, storage and transportation. This progress relies on our ability to optimize the properties of these compounds, e.g., to make a room-temperature superconductor or a ferromagnetic semiconductor. Optimization of their properties, in turn, requires a complete theoretical understanding of these materials. Unfortunately, these compounds display complex emergent phenomena and competing phases which inhibits the use of conventional reductionist theory, so that progress will only be achieved with significant computational modeling

Strongly correlated materials are described by self-consistent field theories, which now may be parameterized by numerical calculations. The latter are used to provide complete information about the material on the short length scales while the former provides the intermediate and long length scale information. In general, such multiscale methods are more accurate when they are parameterized by *both* one (e.g., photoemission spectra) and two-particle properties (e.g., susceptibilities to different external fields). However, until recently, the solution of a complete set of two-particle equations has not been possible, since it involves the rotation and contraction of large rank-three tensors. Consider a single-band system with N=40 sites and L=100 time slices. The corresponding two-particle rank-three tensors (susceptibilities, vertices, etc.) require nearly 2TB of storage each.

However, early petascale systems, such as the national leadership class machines at ORNL (Jaguar) and on the NSF Teragrid (Kraken) will allow us to store this needed data. But, efficient computational methods for rank-three tensor rotation and contraction are needed to solve the self-consistent field theory equations. The development of low-level high-performance parallel programs for them is usually very tedious and time consuming. We have developed techniques in the Tensor Contraction Engine project to address the following: (i) use algebraic transformations to reduce the number of operations; (ii) minimize the storage requirements to fit the computation within the storage disk limits by using compiler transformations. Additional specific techniques are need to: (i) reduce memory access costs by minimizing disk-to-memory and memory-to-cache traffic; (ii) enhance parallelism, and (iii) develop a strategy to call BLAS library to implement tensor operations.

A part of this research is funded by a DOE SciDAC grant and computer time is provided by a large INCITE allocation on Jaguar and a TeraGrid allocation on Kraken. Computer resources available for this project include more than 25M hours of CPU time on petascale machines. We are presently writing an NSF CDI proposal to support this effort. The purpose of this request is to acquire the resources needed to extend this collaboration to involve additional CCT faculty and LI researchers, thereby building a truly Louisiana focused interdisciplinary collaboration. The CS will collaborate with us, the students and postdocs in our groups, and researchers throughout the state involved in a recent EPSCoR application. The CS will be a coauthor/coinvestigator on related publications and grant applications.

Required Effort. Roughly 6 months of the CS's time will be required to integrate the Tensor Contraction Engine into existing massively parallel codes, optimize the codes, and raise the level of abstraction used in order to create portable, modular and sustainable software.

How the project will benefit the LI. It will make the CCT and LI more visible on national leadership class machines thereby greatly enhancing their national and international exposure. Jarrell and Moreno recently moved to LSU, allowing this SciDAC project to acquire an LA focus. It will generate a greatly improved publically available code in an important area of research for both new devices and energy technology.

LI Proposal: Parallel Algorithms for Large Scale Data Clustering

Dr. Vijay Raghavan, Dr. Ryan Benton, Center for Advanced Computer Studies, UL Lafayette
Dr. Raju Gottumukkala, Dr. Ramesh Kolluru, NIMSAT Institute, UL Lafayette
Dr. Box Leangsuksun, Department of Computer Science, Louisiana Tech University

Clustering attempts to group similar objects together based on certain similarity. Traditional clustering algorithms were originally designed for small data sets. Given the exponential growth of data (text, images and video) obtained from advanced instruments, sensors and the Internet, the machine learning communities are exploring ways to refactor existing learning techniques to exploit the computational opportunities found through parallel processing (via cores, clusters, and clouds). In addition, it is known that no single clustering algorithm is capable of successfully grouping all types of objects; each clustering algorithm has a 'bias' that shapes how objects are perceived and grouped. A solution is to generate several sets of clusters via different techniques and select the best solution. This assumes that the user has enough knowledge to determine what the best solution is. Since this is rarely true, the use of ensembles of clusters has been proposed; ensembles of clusters begin with the generation of several different sets of clusters. Then, the predictions of the clusters are then combined (similar to merging the predictions of experts) into a final outcome. Traditionally, using ensembles is quite expensive; a potential solution is via the use of distributed computing to mitigate the impact.

One application lies in finding spatial regions in the brain that characterize stages of dementia. In this case, Positron Emission Tomography (PET) imagery is converted into a series of 3-D points, with each point representing metabolic activity. By grouping points together, based on activity and location, one could isolate regions of the brain that are indicative of progression of dementia. Other dementia-related applications lie in clustering information gathered through exams such as Functional Assessment Exam and the Mini-Mental State Exam. In addition to dementia, other target clustering applications include the spatiotemporal clustering of satellite imagery for disaster impact and characterization of highway accident data.

Goals

The main goal of this project is to investigate optimal approaches to parallelize various clustering and association mining algorithms both on LONI and a prototype cloud cluster at the Center for Advanced Computing Center (CACS). These algorithms help multiple interdisciplinary projects including Alzheimer's Disease Neuro Imaging Initiative (ADNI) datasets for characterizing and predicting dementia, spatiotemporal clustering of geospatial imagery and text mining of web data.

Effort Requested of LI Computational Scientist

We request 30 hours per month of effort for one year (FTE of 2 months) of the LONI Computational Scientist, Dr. Raju Gottumukkala's for this project. The LONI Computational Scientist would help with investigating the best approaches to improve the performance of various data mining algorithms using MPI, OpenMP, and Map/Reduce frameworks.

Benefit to LONI Institute

The research project will benefit multiple projects. In general the developed applications will provide the MPI/OpenMP implementations of data mining algorithms for LONI users upon validation. This project will also potentially advance the LONI infrastructure to support data parallelization using Map/Reduce frameworks such as Hadoop.

Parallel Optimization Algorithms for Disaster Management

Dr. Ramesh Kolluru, Dr. Mark Smith, Dr. N. Raju Gottumukkala, NIMSAT Institute, UL Lafayette

Dr. Baker Kearfott, Department of Applied Mathematics, UL Lafayette

Dr. Dileep Sule, Department of Industrial Engineering, Louisiana Tech University, Ruston

Background

Optimization refers to comparison of a number of solutions before arriving at the optimal solution. With the increase in the number of variables and the number of objectives that have to be satisfied at the same time, the evaluation of a solution can be time consuming because an algorithm has to consider all possible alternatives. Decision support applications for emergency management are time critical and need to be highly interactive. Therefore, parallelizing various optimization algorithms that are applicable in various decision support tools would significantly reduce the computation time. Existing GIS based tools like ESRI's ArcMap, Google Earth, and Hazards US (Hazus) used by emergency managers and first responders do not support analysis of large-scale and complex spatiotemporal datasets or exhaustive planning simulations. The effectiveness of disaster response and decisions are noticeable post-response when major catastrophes have already happened, hundreds of thousands of people were stranded in traffic due to unavailability of gas, and millions of dollars were spent in mismanagement of resources or not having prioritized the recovery of critical infrastructures.

Goals

The NIMSAT Institute works on multiple research and development projects from multiple emergency management agencies including the Louisiana's Governors' Office of Homeland Security (GOHSEP), Department of Natural Resources (DNR) and Department of Homeland Security (DHS). These projects have various components that require developing optimization algorithms for enhancing disaster preparedness and response. The main goal of this project is to develop parallel optimization algorithms on LONI for enhancing various disaster management applications such as evacuation models, site selection algorithms and infrastructure interdependency analysis.

Effort Requested of LI Computational Scientist

We request 6 months of FTE for the LONI Computational Scientist, Dr. Raju Gottumukkala's time for developing algorithms and parallelizing them on LONI for multiple projects at the NIMSAT Institute. The institute was recently funded through the Louisiana's DNR to develop a fuel demand model for evacuations through analyzing the historical traffic patterns, real time traffic feeds and assessing the evacuation behavior. Raju has been involved with the development of the fuel demand model and would enhance it and eventually investigate approaches to improve the performance of the algorithm by running this algorithm on LONI.

Benefits to the LONI Institute

This project involves researchers from multiple disciplines including transportation modeling, computer science, industrial engineering and applied mathematics. This project also offers a unique opportunity to improve the decision support tools of emergency managers through cyberinfrastructure as most HPC projects in the nation have been about hazard or weather prediction. In addition to current funding, this project has a great potential for federal funding from NSF, DHS and FEMA.

iLevee: Intelligent Flood Protection Monitoring, Warning and Response System

Dr. Ramesh Kolluru, Mr. Dean Mallory, Dr. N. Raju Gottumukkala,
NIMSAT Institute, University of Louisiana at Lafayette
Dr. Box Leangsuksun, Computer Science Department, Louisiana Tech University
Dr. Honggao Liu, Director of HPC, Louisiana State University, Baton Rouge, LA

Background

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 under its responsibility. In this effort, DNR has funded a pilot implementation of this project through a collaborative effort of multiple organizations including Geocomp Corporation, PB Americas, Shannon & Wilson, James Lee Witt Associates, NIMSAT Institute at the University of Louisiana at Lafayette, SMARTEC and TIE Technologies.

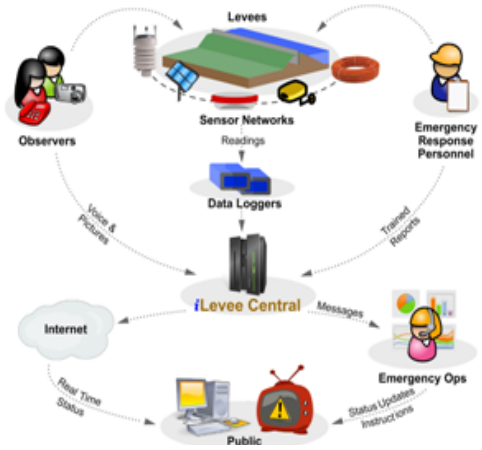


Figure 1. Concept of the iLevee System (Taken from the Proposal)

Project Description

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.

Time for LI Computational Scientist

The primary objective of this project is to develop and deploy an iLevee Central system that runs on LONI and UCSD. Dr. Gottumukkala was involved in writing the proposal and we request FTE of 6 months of the LONI Computational Scientist, Dr. Raju Gottumukkala's time for the next one year for the iLevee project. Dr. Gottumukkala will work with various faculty and staff from NIMSAT Institute and LONI Institute to design a highly-available iLevee Central system that will be deployed on LONI and parallelize various data processing and computation modules that will improve the response time of the iLevee Central.

Benefit to LONI

This project will be a collaborative effort across multiple universities and industry and an opportunity for the state's investements on LONI to be utilized for the state's emergency management efforts.

High Performance Computational Biology and Material Science Projects at Southern University HPC-BMSL Lab (FY: 2010~2011)

PI: Dr. Ebrahim S. Khosravi (Chair of Computer Science, SU)
Co-PI: Seung-Jong Park (Computer Science, LSU)
Co-PI: Marcia Newcomer (Biology, LSU)
Co-PI: Shengmin Guo (Mechanical Engineering, LSU)
Co-PI: Dr. Shuju Bai (Computer Science, SU)
Co-PI: Dr. Shizhong Yang (Computer Science and LONI CS)

The High Performance Computational Biology and Material Science Lab (HPC-BMSL) at Computer Science Department of Southern University proposes to perform 4 sub-projects in Fiscal year 2010(Mar. 2010 ~ Feb. 2011). The objectives of the projects are, (a). to setup and test a CRON high speed optical fiber network testbed at SU; (b) to perform ligand docking and QM/MM simulation of AA/8R-LOX, to understand and predict the electronic, optical, magnetic, and structural properties of the selected novel electronic materials; (c) to provide an infra-structured platform for systematically mentoring and training of under-graduate, graduate students, and post-doctors at Southern University and A & M College.

Dr. E. Khosravi will supervise all of the four proposed projects. The four sub-projects will synergistically address complementary tasks to dramatically enhancing our fundamental knowledge and practical applications in the biochemistry, drug design, and nano-size material science. The four research subprojects and proposed time are:
(1). The CRON high speed optical network testbed setup and testing by Dr. E. Khosravi, S. Park and S. Yang; (3 month).
(2). AA/8R-LOX docking and QM/MM simulation by Dr. Shuju Bai, Marcia Newcomer, E. Khosravi, and Shizhong Yang; (3 month).
(3). Ta doped ZrO_2 Thermal Barrier Coating (TBC) MD simulation by Dr. Shengmin Guo, E. Khosravi, and S. Yang; (3 month)
(4). Graduate, undergraduate students, and faculty HPC related research training. (1 month)

Project 1: The CRON high speed optical network testbed setup and testing
Dr. Khosravi and Dr. Park are funded by a NSF project CRON throught LSU CCT. Dr. Yang will be responsible for the high speed optical fiber network setup, including purchasing the workstation (Sun Microsystems), fiber, and network PCI card, setup the workstation and fiber network connection through the P5 LONI machine's optical port, test the connection and communication. Dr. Yang will also assist in the code developing and student training.

Project 2: AA/8R-LOX docking and QM/MM simulation
Dr. Shuju Bai and Dr. Newcomer will be the sub-project PIs. In this project Dr. Yang will be working on the AA/8R-LOX docking and QM/MM simulation. The ICM-Pro and Q-Chem will be utilized to simulate the docking site and chemical active site of the protein. The results will provide basic information for the drug design.

Project 3: Ta doped ZrO_2 Thermal Barrier Coating (TBC) MD simulation
Dr. Shengmin Guo, Shizhong Yang, E. Khosravi, and graduate students will perform ab initio MD simulation of Ta doped Yttrium (1:1) doped ZrO_2 (YSZ). This will extend current NASA-

EPSCoR supported TBC project and to enhance the closely collaboration with NASA Glenn Research Center where the Ta doped YSZ experiments are ongoing. All the simulations will be performed on LONI machines.

Project 4: Graduate, undergraduate students, and faculty HPC related research training
Southern University and A & M College is a traditionally large HBCU institution. Dr. Yang and LONI staff at SU will host an annual LONI HPC training session. Minority student and faculty will be trained by intimately engaging them in the training activities. Under Dr. Yang's funding supports, he will also support two graduate students to do the above proposed projects.

The PI, Dr. Khosravi, Chair of the Computer Science Department and LONI SU Co-PI, is currently funded by Navy, Raytheon, NSF, BoR, NIH, and NGA. Three Co-PIs, Drs. Park, Newcomer, and Guo from LSU are faculties who are experts at Computer Science, Biology, and Mechanical Engineering fields respectively. Support to the proposed LONI projects would generate new opportunities to attract more talented faculties, post-doctors, and students, secure more federal and industry funds, which without doubt fits into SU and LONI's long term development strategy.

Simulating Larval Dispersal in the Northern Gulf of Mexico

PIs: Caz Taylor (Assistant Professor, CCS & EEB, Tulane University), Richard Condrey (Associate Professor, OCS & ACE, Louisiana State University), Woody Nero (Oceanographer, NOAA National Marine Fisheries Service & Northern Gulf Institute), Erin Grey (Postdoctoral Researcher, EEB, Tulane University), Carey Gelpi (PhD Student, OCS & ACE, Louisiana State University)

Background: Commercial fishing in the Gulf of Mexico generates more than $900 million per year, representing approximately 25% of fishing revenue in the U.S. [1]. Many of the organisms fished, such as crabs and shrimps, disperse as small larvae that drift in near-shore currents. Understanding this dispersal phase is crucial for developing predictive population models. Yet such understanding has proven difficult because near-shore currents in the Gulf are influenced heavily by winds and tides [2] and because larvae often exhibit vertical swimming behaviors that can significantly alter their horizontal trajectories [3].

Project Proposal: Recently, the Naval Research Lab has developed the Northern Gulf of Mexico Ocean Nowcast/Forecast System (NGOMNFS) which incorporates wind and tide data to resolve near-shore circulation patterns at a 1.9 km, hourly scale that is sufficient for tracking larvae [4]. We proposed to simulate larval dispersal in the northern Gulf of Mexico by running a larval-behavior model through the archived NGOMNFS database (~1TB). The behavior model was written by Woody Nero at NOAA in Matlab and was parameterized for brown shrimp larvae. The current model is slow, taking 1 hour to simulate one night's release and dispersal of 500 larvae and 15 days to evaluate one year. We will develop more general and efficient software that can be easily modified to simulate the dispersal of species with different larval behaviors, and we will parallelize the model to run on the LONI cluster to speed up simulations. Postdoctoral researcher Erin Grey will use this resource to estimate blue crab dispersal for a dynamic population model for this species, Dr. Richard Condrey and Carey Gelpi will use it to look at blue crab dispersal from offshore shoals, and Woody Nero will use it to continue his research on brown shrimp dispersal. Additionally, the software will be made freely available through LONI and the Northern Gulf Institute, which is a consortium of universities led by Mississippi State University that seeks to integrate coastal science research.

Effort Requested: We request 1 month of full-time effort from a LONI Institute computational scientist who could assist Erin Grey and Carey Gelpi in compiling the larval-tracking code and then parallelizing it to run on the LONI cluster. Dr. Hideki Fujioka has already expressed willingness to work on this project, and his proximity to Dr. Grey at Tulane University would be convenient. We would, however, appreciate help from any of LONI's computational scientists.

Benefit to LONI Institute: This project represents collaboration between Tulane University, Louisiana State University, the NOAA and the Northern Gulf Institute, and would thus help LONI achieve its goal of fostering research collaborations. Furthermore, the end-result of this will be efficient, freely-available larval-tracking software that will encourage a variety of coastal scientists to utilize LONI's computational resources. Given the importance of larval dispersal to the majority of estuarine species, this LONI-based product will also greatly contribute to fisheries and ecosystem management in the Gulf of Mexico.

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Computational Infrastructure for Genome-wide Change Point Analysis at Basewise Resolution and Transcriptome Characterization on the Isoform Level

Dongxiao □hu (UNO), □hiyu □hao (UNO), □un □hang (□avier) and Erik Flemington (Tulane)

1. Computational Infrastructure for Genome-wide Change Point Analysis at Basewise Resolution

Our goal is to develop a computational infrastructure for performing genome-wide change point analysis with base-wise resolution. Our experimental system is the detection of miRNA targets on the genome scale. miRNA is a recently discovered gene regulation mechanism that down-regulates gene transcription and translation by Watson-Crick paring with target sites. More than 80□ of human diseases have been shown to be intimately related to miRNAs. miRNA target prediction on the base-wise resolution has become a promising way to discover disease genes.

Using the very high-end sequencing technology, next generation sequencing, we have identified functional target genes of the human microRNA, miR-155, a highly implicated oncogenic microRNA in a number of immune cell cancers. A genome-scale analysis on the basewise resolution will be needed to discover more novel miRNA targets. Algorithmically, we first align the short reads characterizing the transcriptome to the reference genome sequence, and then calculate genomic coverage. The targets are predicted by abrupt drop outs of the coverage on the 3'-UnTranslated Region (UTR), called by low values of Schwarz Information Criteria (SIC) from a Change Point Analysis. The computational complexity of SIC based change point analysis at basewise resolution is $O(N^2 \log N)$□therefore, for $N = 3.2 \times 10^9$ potential change points in human genome, the number of calculations needed is easily to reach 10^{20} which takes hundreds of billions of seconds on a CPU with a few giga flops of computation power.

We propose to develop a computational infrastructure to run the change point analysis at basewise resolution for the human genome. The infrastructure is parallel computing in nature, since the problem size makes it infeasible on any single workstation. In case the base-wise change point analysis becomes intractable even in parallel, alternatively, we will perform a similar change point analysis using the same score and search strategy but at a lower resolution, e.g. exon-wise or gene-wise change point analysis. It will dramatically decrease the problem size *N* to $10^{5.}$

2. Computational Characterization of Transcriptome on the Isoform Level

Our goal is to develop a computational infrastructure for automatic characterization of transcriptomes on the splicing isoform level. Due to inherent limitations of hybridization based expression microarray technology, it only allows for the characterization of transcriptomes at the gene level. However, in the real biological system, the ultimate effectors on the transcription level are the splicing isoforms. One gene can be alternatively spliced into different isoforms of transcripts in different tissues. Despite providing output on overall gene expression, isoform analysis using microarray data is computationally inaccessible.

The advent of a very high-end technology, next generation sequencing, has provided new opportunities to solve this problem. It provides more accurate quantitative data and it provides additional information that allows the characterization of a transcriptome at the isoform level. We have designed an iterative algorithm to detect splicing isoforms using short reads originating both from exons and exon-exon junctions. More formally, assume $i = (1,2 \ldots, \mathrm{N})$ is the short read (row) index, $j = (1,2 \ldots, \mathrm{M})$ is the isoform (column) index and $\emptyset = (p_1, p_2, \ldots, p_M)$, where p_j is the mixture proportion for the isoform j. Initializing all the compatible p_j to be the same, and add up to 1, i.e. $\sum_{j=1}^{M} p_j I_j = 1$, where I_j is the indicator having value of 1 if the jth isoform is compatible, 0 otherwise. The proposed Expectation Maximization (EM) type algorithm is as follows□E-step□$z_{i,j}^{(k+1)} = \frac{y_{i,j} p_j^{(k)}}{\sum_{j=1}^{M} y_{i,j} p_j^k}, \forall i, j$. M-step□Let $n_j^{(k+1)} \square \sum_{i=1}^{N} z_{i,j}^{(k+1)}, \forall j$, $p_j^{(k+1)} \square \frac{n_j^{(k+1)}}{N}, \forall j$. In a proof-of-principle study, we have shown that our algorithm is able to accurately identify all splicing isoforms in mouse liver, brain and muscle.

The real challenge comes in the computational side in that the same iterative algorithm must be applied to a total of 22,000 genes annotated in human genome. The computational complexity of each gene is $O(M^2N)$, where M is typically 50 to a few hundreds, and theoretically N can be exponential to M. 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.

3. Benefits to LONI users, Louisiana researchers and more

This project will benefit LONI by fostering collaborative efforts from multiple Louisiana institutors in their efforts in multidisciplinary cancer research. The proposed computational infrastructure is quite general and widely applicable to diverse tissues and biological conditions wherever the Next Generation Sequencing data is available. For example, detection of chromosome copy number changes, *de novo* gene prediction etc. 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.

□. PIs' roles and request for the FTE of Dr. □hao

We request six months of full time effort of Dr. □hao to develop a parallel algorithm for the proposed works and implement it on the LONI clusters. We have a multidisciplinary team of scientists involved in the project. Drs. □hao and □hu will collaborate on the algorithmic and computational side of this project to run the change point analysis and the transcriptome characterization on the LONI clusters while minimizing the use for CPU time. Dr. Flemington will provide expert opinions and insights from biological domains to interpret the findings. Dr. □hang will also collaborate on the computational side and assist the outreach to researchers and educators at □avier University, a Historically Black Colleges and Universities (HBCU).

Surface plasmons in metal/semiconductor composites and devices

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

***Background*:** The inhomogeneous metal/semiconductor composites are nanoscopic artificial materials that have unique geometrical and optical properties. Under electromagnetic wave illumination these complex materials manifest energy localization in very small spatial areas (a few nanometers) and giant enhancement of the local field intensities, which correspond to excitation of localized surface plasmon (SP) modes. At critical metal concentrations, the random films are inhomogeneous and self-similar (fractal) on any length-scale. Thus, for any incident wavelength resonating clusters exist in the composite. Such broad frequency response results in anomalous optical properties including extraordinary absorption and enhancement of nonlinear optical processes such as Surface Enhanced Raman Scattering (SERS), high order frequency generation, etc. The unique properties of the percolating films make them ideal not only for fundamental studies of light-matter interaction in disordered systems, but also for a wide range of applications in biological sensing and spectroscopy, fast optical devices, surface science, and condensed matter physics.

Proposed research: **1.** ***Numerical methods in nanoplasmonics*:** As part of this proposal we first seek to rewrite the existing FDFD codes in parallel and develop novel, highly efficient numerical methods for calculating the electromagnetic (EM) response of 2D and 3D inhomogeneous systems of metal/semiconductor nanoparticles. Additionally, we intend to use a 'memoization' 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). Successful development of the numerical codes will 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 will allow for a first time to study local and macroscopic response of real size systems and compare with existing experimental data. The developed numerical codes could be effectively applied to investigate large variety of strongly interactive, sub-wavelength ensembles of particles, including dense semiconductor quantum dots systems, periodic arrays with tunable optical properties, photonic nano-circuits and optical switches. **2.** ***SP transistor*:** Relying on the above surface plasmon related studies, 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. 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. 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.

Impact of the proposed research: The proposed research will lead to development of numerical and analytical tools for solving highly complicated problems of EM interaction with complex media. Those methods will answer standing fundamental questions concerning the nature of collective electronic excitations in metal-dielectric composites. Due to the inhomogeneous nature of the problem it is crucial that very large system sizes are investigated. Such systems cannot be studied with average computational facilities and utilizing the LONI recourses will allow to traverse new regimes of operation that have been a mystery for the last 50 years. Successful realization of the project will help to establish the LONI Institute as a top center for computational electromagnetism. Furthermore, this project will focus 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 but also with other national universities including groups at UC Berkeley (Dr. X. Zhang), and Yale University (Dr. Hui Cao). The first part of this project has been included into a RCS proposal submitted on Nov. 4 to the Louisiana Board of Regents, while the SPT data will be used in a proposal to be submitted to the NSF-EPM program. The total workloads for the LI faculty and CS are 3 FTE-months per year, for total duration of the proposal of 1.5 years and expected supercomputer time allocation of 50K SUs. Also, the LI faculty will provide a PC workstation and a graduate student to work full time on the project, which will also be the subject of the student PhD thesis.

Date: 12/10/09

Improving Antibody Design by Structure Prediction, SCOP Classification and Protein - Protein Docking

Seth Pincus (spincus@chnola-research.org)
Research Institute for Children, Children's Hospital New Orleans & Louisiana State University Health Sciences Center

Zhiyu Zhao (sylvia@cs.uno.edu)
LONI Institute & Department of Computer Science, University of New Orleans

Bin Fu (binfu@cs.panam.edu)
Department of Computer Science, University of Texas – Pan American

We propose to use a structure similarity search tool that we have developed in conjunction with existing structure prediction and protein - protein docking tools to improve the structural design of an antibody. We will be able to test experimentally the computational prediction of improved design by altering the amino acid sequence and determining whether the resulting antibody has the expected immunological characteristics. Antibodies can be used for molecular measurement and to treat diseases. The efficacy of antibodies is related to binding affinity. The software we propose to develop will allow computational prediction of higher affinity antibodies; such tools are of potential value to biotechnology and pharmaceutical companies.

The computational improvement process will be automatic. It will take amino acid sequences of variable regions in an antibody as input, and output improved structures predicted to interact better with antigen. The improved antibodies, which belong to the same Structural Classification of Proteins (SCOP) domain, family, or superfamily, are structurally similar to the original one, but with specific amino acid changes. It is these differences that result in a better interaction with antigen. Computationally, our antibody improvement problem is described as: Given amino acid sequences of heavy chain variable region (V_H) and light chain variable region (V_L) in a monoclonal antibody, create *denovo* structures for the antibody complementarity determining regions (CDRs) by finding similar structures in a protein database, engrafting them onto the antibody backbone, and testing them, *in silico*, for docking with the antigen. The improved design of that antibody structure may result in a better binding with its antigen.

Instead of relying merely on sequence similarity search tools such as IgBLAST to find similar amino acid sequences in an antibody, we plan first to use a structure prediction tool to predict the structure of that antibody. Currently there are three antibody-modeling servers on the Internet: the Web Antibody Modeling (WAM), Prediction of Immunoglobulin Structure (PIGS), and RosettaAntibody (command line tool also available). We have requested the installation of Rosetta on Queen Bee. We will investigate the antibody modeling performance of these servers, by testing their predictions with antibodies whose 3D structures are known. We have obtained some preliminary results. See Figure 1 and Figure 2 for antibody modeling results of RosettaAntibody and PIGS based on protein 2DDQ (detailed interpretation of these results and other preliminary results are not presented due to page limitation and can be provided upon request). By comparing the predicted structure to the actual structure, particularly for antibodies similar in sequence to our test antibody, we will choose one as our antibody structure prediction tool. Then, since the predicted antibody structure is new to the Protein Data Bank (PDB) and its SCOP domain, family and superfamily are unknown, we will use the SCOP classification tool that we have developed to predict the class of that structure, and to retrieve from the PDB a set of similar antibody structures that belong to the same class i.e. the same SCOP domain, family or superfamily. Next, we will use a protein - protein docking tool to predict the structure of each antibody - antigen complex and observe changes in the antibody that would result in a better binding.

Figure 1: RosettaAntibody Model Rank 1 vs 2DDQ

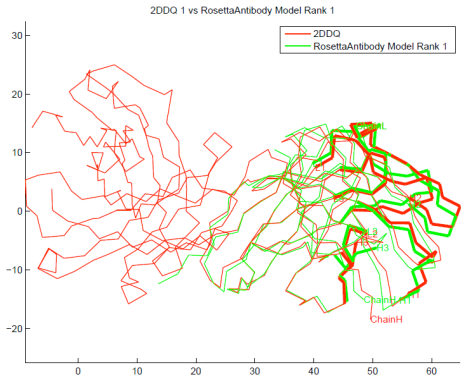
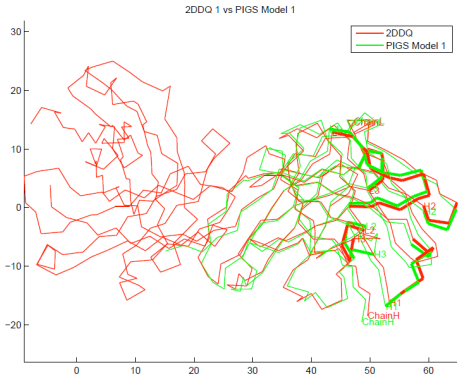


Figure 2: PIGS Model 1 vs 2DDQ



The antibody, RAC18, we will be working with is a well-studied molecule, which binds to the plant toxin ricin, a material of biodefense concern. This antibody has been shown to be of protective efficacy in animal models, even when administered hours after the toxin. We now wish to improve the affinity of this antibody. The amino acid sequences of the heavy and light chain variable regions are known, as are the amino acids that the antibody contacts on the ricin molecule. Once computational predictions have been made regarding specific alterations to improve binding to ricin, we will use genetic engineering technologies to make that antibody and test it to determine if we have improved the affinity of binding to ricin and its protective efficacy *in vivo*.

We request 6 months of full time effort of Dr. Zhiyu Zhao over a one year period to work out preliminary results using existing and homemade software tools. Dr. Zhao will then develop an antibody improvement software tool which automates the above mentioned improvement procedure. All the software development work will be performed on a LONI cluster such as Queen Bee. These specific experiments may significantly improve the function of a clinically important antibody. By addressing this theoretically important issue in a well-characterized experimental system these studies may represent the initial steps in the production of more general tools for enhancing antibody and protein design. The successful prediction of protein improvements by a computational approach would be an important accomplishment in the field of bioinformatics.

In the last a few years, we have successfully developed efficient software for alignment and similarity searches of protein structures with structures in the Protein Data Bank. The proposed project is a continuation of our ongoing development in this field. The next phase of this work is to apply the computational tools to address practical biological problems, such as this one from Dr. Pincus's group. It will also strengthen our ongoing collaboration with Dr. Bin Fu's group, which is focusing on the protein folding problem at the University of Texas-Pan American.

Computational Model of Pulmonary Small Airway Interdependence

Hideki Fujioka[1], David Halpern[2] and Donald P. Gaver[3]
[1]Center for Computational Science, Tulane University
[2]Department of Mathematics, University of Alabama, Tuscaloosa
[3]Biomedical Engineering Department, Tulane University

Project Description

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.

Pulmonary epithelial cells are exposed to mechanical stresses due to the stretch of the surrounding substrate and the motion of thin liquid film over them. There are a number of situations that these stresses becomes excessive, leading to cell damage or death. For example, local reduction of surfactant concentration results in nonuniform deformation of the parenchyma and the airways, and causes high membrane strain and high fluid stress due to high surface tension. Surface tension induces liquid flows, which may cause the lung's airways to close due to the formation of a liquid plug as a result of drainage of the liquid lining coating the airways or collapse of airway due to low pressure in the liquid. Once occluded either by a short plug or an extended collapsed region, the airway must be reopened to maintain ventilation to distal regions of the lung.

Though simplified models of airway closure and reopening phenomena in single airways have led to advances in our understanding of atelectrauma, the effect of the surrounding alveoli and the interdependence of airways on the these phenomena needs to be studied.In this project, we plan to investigate the effect of parenchymal tethering on inflation/deflation mechanisms of atelectic regions of the lung. This may yield improved technologies for reducing the morbidity and mortality associated with respiratory distress syndrome and ventilator-induced lung injury.

Employing our previous method to solve the fluid mechanics[1,2], we modify the model to add parenchymal effect. A truncated-octahedron alveolus computational model[3] is employed. The displacement based finite element method is used to analyze large deformation of the alveoli surrounding airway models. The code is parallelized using MPI and PetSc library. We would like to request 6 months of an FTE of LONI Institute Computational Scientist who is experienced in pulmonary mechanics and computational modeling. This research will enhance collaboration between the Center of Computational Science and faculty members and students in the department of Biomedical Engineering at Tulane.

Benefit to LONI Institute

This project would develop a expertise in the multi-scale modeling of pulmonary system and show LI's capabilities of large scale computational modeling for fluid and solid mechanics.

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Project: Thermal Modeling and Thermo-mechanical Modeling of Thermal Barrier Coatings (TBCs) using Ansys Fluent Commercial Package

Stephen Akwaboa
Department of Mechanical Engineering
Southern University and A&M College
Baton Rouge, LA 70813
stephenakwaboa@engr.subr.edu

Thermal barrier coatings (TBCs) are used in gas turbine engines to achieve higher turbine inlet temperatures (TITs), improve turbine operating temperatures, reduce fuel consumption, increase components lives and thus lead to better turbine efficiency. Yttria-stabilized zirconia (YSZ), is an ideal candidate for TBCs as it has good thermal shock resistance, high thermal stability, low density, and low thermal conductivity. Traditionally, there are two main methods of fabricating TBCs: air plasma spray (APS) TBCs and electron beam physical vapor deposition (EBPVD) TBCs. The ability of TBCs to offer thermal protections to metallic substrates, to a large extent, depends on their thermophysical properties (thermal diffusivity, thermal conductivity and specific heat capacity) as well as their porosity. We have purchased laser flashline equipment (FL 5000) from Anter Corporation to characterize the thermophysical properties at high temperatures (up to 1300 ^{o}C). The porosity of the samples are measured using Poremaster, a mercury porosimetry equipment manufactured by Quantachrome Incorporated. Operating modern turbines at high temperatures is crucial to most turbine researchers since it is the main potential source of improving engine efficiency. In order to avoid overheating of the metallic components and also to prevent corrosion and oxidation at elevated temperatures, thermal barrier coatings (TBCs) are the ultimate choice. By using TBCs, turbine inlet temperature can be increased by 200°C. It is also known that the use of TBCs promotes enhanced component life, reduces fuel cost, and combustion gases emitted into the atmosphere.

Our ongoing research involves the use of TBCs on superalloy IN 738 substrate materials for elevated temperature gas turbine applications. In principle the focus of our research involve thermophysical properties characterization of TBCs, thermo-mechanical analyses of the TBCs and micro-scale thermal modeling of in-service performance studies of the TBCs. By using the thermophysical properties as inputs to the thermal modeling in Ansys Fluent CFD Commercial package, the temperature distribution in the metal substrate and the composite TBCs are determined. The Fluent solution is exported into Ansys to perform the thermomechanical anaylsis utilizing the temperature distribution as thermal loads. Analysis in Ansys gives the thermal stress distribution in the metal substrate as well as the in-plane stresses at the various interfaces of the TBC system (top coat/TGO, TGO/bond coat and bond coat/ substrate interfaces) which are crucial in identifying high stress areas in the TBC system.

Even though we have purchased Ansys Fluent products which are used to do most of our thermal and structural modeling work, we are constrained by the number of nodes we can use for our analysis. Ansys , for instance, allows only 256 kilo-nodes for its structural analysis package. This cap on nodes greatly compromises the quality of work that we can produce and publish. We need high resolution models in Fluent and Ansys to be able to obtain good solutions with high reliability. This means we need computers with superior computing power, hence my request for this allocation so good quality work can be produced for publications in a timely manner. We request the services of a Computational Scientist in Spring of 2010 (50 hrs) to help us to run our code on the supercomputers for quick solutions.

Large-Scale First Principles Computation and Simulation of Catalytic Properties of Nitrogen Doped Carbon Nanotubes for Dioxygen Reduction
(A LONI Proposal for FY 2010 - 2011)

PI: Dr. Guang-Lin Zhao, Professor, Department of Physics, Southern University and A & M College, Baton Rouge, Louisiana 70813. (Phone) 225-771-4491; (fax) 225-771-2310; (email) Guang-Lin_Zhao@subr.edu.
Co-PI: Dr. Ebrahim Khosravi, Professor, Computer Science Department, Southern University and A & M College, Baton Rouge, Louisiana 70813
Co-PI: Dr. Shizhong Yang, Computational Scientist and Assistant Professor, Computer Science Department, Southern University and A & M College and LONI CS, Baton Rouge, Louisiana 70813

Proposal Description

We propose to perform first principles density functional calculations for the catalytic properties of nitrogen doped carbon nanotubes (CNTs) for dioxygen reduction, by requesting **two month**s of Dr. Shizhong Yang's research time in fiscal year 2010-2011 (Mar. 2010 - Feb. 2011). 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.[1] 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.[2,3]

In 2006, Ozkan and coworkers reported that nitrogen-containing nanostructured carbons and nanotubes have promising catalytic activity towards ORR.[4, 5] 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.[6] 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*.[7] 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.[8]

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.

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.

Corresponding PI's email address: Guang-Lin_Zhao@subr.edu

Co-PI's email addresses: Ebrahim_Khosravi@subr.edu, Shizhong_yang@subr.edu

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Leveraging LONI Workflow Developments onto TERAGRID To Enable High Performance High Throughput Molecular Dynamics Simulations.

PI: **Thomas C. Bishop (CCS, Tulane University)**

bishop@tulane.edu

504-862-3370

Senior Investigators: Joohyun Kim and Nayong(CCT, LSU)

Requested: LI Computational Scientists (CSs) Time: 6 months FTE-months

Project Description:

In an NIH funded study (R01GM076356) Bishop's goal is to investigate sequence dependent variations in nucleosome stability using molecular dynamics simulation techniques. Nucleosomes are the fundamental structural unit of chromatin and can be formed from any 146 basepair segment of DNA. In theory there are some 4^{146} possible sequences of nucleosomal DNA. In practice the ~12 million basepairs in the yeast genome position only about 60,000 nucleosomes (Jiang, et al., 2009). The degree of positioning ranges from highly positioned to nearly random positioning. Unfortunately, all available x-ray structures of the nucleosome have utilized nearly the same 146bp sequence of DNA (Luger, et al., 1997). We therefore have limited information on sequence induced structural variations in the nucleosome superhelix.

Progress to Date:

In order to investigate sequence dependencies, we implemented with the support of LI staff, a high-performance high-throughput molecular dynamics work flow on LONI (Bishop, 2010). Our workflow strategy was inspired by NAMD-G (Gower, et al., 2006), but was structured so as to take advantage of Louisiana Optical Network Initiative (LONI) resources. We used 4 LONI machines and Petashare (Wang, et al., 2009) to accomplish these simulations by farming them out in groups of 4 to Oliver, Louie, Poseidon, and Painter. Each simulation utilized 64cores (16nodes) and all tasks were run in 1ns increments (approx. 16hrs run time per ns of simulation). In total there were 16*16 = 256 tasks to be completed. Each task began by fetching via Petashare's pget command the necessary initial coordinates, velocities and parameter files from Petashare and ended by depositing the simulation's outputs (extended system file, final coordinates, velocities, trajectory and velocity files) into Petashare via the pput command. During run time trajectory data was copied on a daily basis from Petashare to Bishop's local computing resources for purpose of analysis and visualization. This avoided a lengthy post-production trajectory transfer. In this manner we were able to complete all simulation tasks during two separate 10 day periods. The first period produced 8ns for each of the 16 systems, and the second period produced an additional 8ns. This workflow enabled us to efficiently utilize nearly 300,000SUs at 4 different LONI sites (sometimes concurrently), and manage approximately 1.5Tb of data via PetaShare. However it still required significant user intervention and manual monitoring of progress.

Need for LI Support:

Based on results from this LONI study of 16 nucleosomes, we were recently awarded a TERAGRID allocation (8,000,000SU) to conduct a larger study that is expect to produce some 40Tb of data. The TERAGRID effort requires that we port our LONI workflow to the TERAGRID environment and that we further automate the workflow. Our workflow makes use of LONI's PetaShare resources and requires advanced scheduling capabilities. Both Petashare and the scheduling tools function differently in the LONI environment than in the TERAGRID environment. Thus developing a workflow solution that works optimally in both the LONI and TERAGRID environments requires collaboration between experts with knowledge and mastery of each.
From a broader perspective developing these tools provides an important/critical bridge between LONI and TERAGRID usage scenarios. The overall goal is to leverage LONI developments efforts for achieving high-performance high throughput molecular dynamics simulations onto the TERAGRID in such a away that we and other users can realize a lower time-to-solution by effectively managing distributed resources where ever they may reside. Molecular dynamics studies are historically the largest consumer of supercomputer resources thus any tools developed for this project will have a significant impact on both LONI and TERAGRID users.

Effort Requested and Involvement of Computational Scientists:

We estimate this will require 6 months of FTE.

Benefit to LONI Institute:

Advanced User Support was requested in Bishop's TERAGRID allocation request. The award received the highest recommendation for AUS possible. Thus LI support for this project provides a unique opportunity for LI and AUS personnel to collaboration in leveraging technology developed on LONI onto the TERAGRID and thereby demonstrate proof-of-concept in the LONI-TERAGRID development cycle.

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A LEARNING MACHINE TOOL FOR LARGE-SCALE SOLVERS ON PARALLEL COMPUTERS

BY ABDELKADER BAGGAG

Context and Summary of the Project

In large-scale scientific and engineering applications, such as the simulations of complex phenomena that span multiple length and time scales, computational fluid dynamics, and environmental simulations, several parameters, whether related to the grid or to the solver, must be fine-tuned to achieve accurate and realistic results. There is no theoretical method to estimate the “optimal” values of these parameters, or the trade-offs between them, and hence they are generally suggested by the user after a long and tedious training based on trial-and-error. On average, it might take days for an experienced user, and up to weeks for a new user, to find the appropriate parameters for a new geometry; and after acquiring an extensive experience, e.g. while doing their research as students or post-docs, this expertise is gone as soon as the researchers leave the lab, and it is (again) a new trial-and-error beginning for new users. A remedy to this would be to preserve, *in some sense,* the acquired expertise, which can significantly enhance the performance of the user by reducing the time-to-solution.

Numerous parameters govern the problem resources, and the number of reasonable choices is overwhelming. The grid-related parameters can be the size of the grid, the distribution of the nodes’ density describing the geometry, the elements’ topology, etc. As for the solver-related ones, we cite, in particular, the stabilization method, i.e., the amount of artificial viscosity and the coefficients related to the limiters, the CFL value, and the type of the iterative solver and its associated parameters like the number of Krylov subspaces, the number of Newton iterations, the acceptable tolerance and the time step. Other qualitative parameters also influence the quest for the “best” solution, depending on whether the physical problem is viscous, inviscid, and laminar or turbulent flows.

It is thus clear that the task of choosing the “best” set of parameters, which combine also memory capacity and execution time, is daunting, and can change according to the geometry, the code implementation, or the available computing resources (serial vs. parallel).

We propose a “learning machine” that is capable to predict and select the “optimal” parameters to match the problem attributes and the new geometry. The learning process will be achieved on a database which will be built progressively by different users. As a consequence of this process, the training of the users and the acquired expertise will be shared and preserved.

The proposed approach would be to use machine learning algorithms to generate functions that map geometries and physical problems to suitable parameters. The mapping function consists of two parts, namely a *feature extractor* and a *classifier*. The set of features is designed to capture the characteristics of the problem (quantitative and qualitative), as precisely as possible. And the classifier maps the given feature values to a choice of appropriate parameters.

We design the feature extractor, and a database is then built progressively and improved upon by the users according to a well-defined protocol. And to construct the classifier, the learning algorithm receives as input a *training set*. The training set contains information about resources of prime importance, including the details of the parameters required to solve the benchmarking problems, with the implicit assumption that the algorithm that performs well on the *testing set*,

will perform well on a new, yet unseen, set, i.e., the generalization capability of the learning machine.

Existing approaches to machine learning and pattern recognition suggest separating feature selection from the construction of the classifier, to avoid *over-fitting*; and a plethora of techniques can be found in the literature. However, these techniques are (generally) application-dependent, and the selection of an efficient classifier is not an easy task due to the complexity of the problem.

We suggest investigating Support Vector Machines (SVMs) and Hidden Markov Methods (HMMs), which proved to be resilient with respect to over-fitting, combined with feature optimization techniques, such as Bayesian approaches, and Genetics Algorithms.

While the topic of "machine learning" is not new on its own and is closely related to data mining and artificial intelligence, (to our knowledge) it has never been applied to linear system solvers, CFD and environmental applications. Hence, this research project can be viewed as an attempt to *reduce* the need for human intuition by automating certain parts of the simulation, such as the choice of the parameters.

The originality of the proposed research project resides essentially in the development of a "learning machine" as an efficient tool, to be used in large-scale linear system solvers in CFD and environmental applications, for the purpose of *automatically* identifying the most appropriate parameters for the simulation. We are mainly concerned by the efficient development of (parallel) algorithms and techniques that allow computers to "learn." This will be achieved by extracting rules and patterns out of massive (CFD) data sets, and an important challenge that faces this project will be the development of a new formalism to this type of applications.

One month of FTE support from the LONI Institute would be instrumental in setting up the ground work for this project.

Appendix D

LI Graduate Fellows, 2009-2010

Steven Baker, LA Tech

Research:

Nano-composites have many applications in today's society. Through molecular modeling, it is possible to develop an understanding of properties present within a nano-composite. Molecular modeling does require computational resources to be effective. My LONI graduate fellowship has provided me with resources to analyze different composites. Not only have I been provided with excellent computational power, I also have access to programs, like Gaussian, to analyze nano-composites. The properties of interest include electrical, thermal, and structural properties.

The initial thrust has been to see what changes occur to electric properties when functionalizing non-metallic carbon nanotubes (CNT) with Ti molecules. Literature suggests that functionalized non-metallic CNTs should exhibit properties similar to metallic CNT's. However, I have not had any of my simulations converge. I intend to run these same models in Atomistix, an electronic modeling program available on painter.

The eventual goal is to develop a multi-scale model of a nano-composite material that has the ability to provide three separate purposes. The first goal is to provide a protective shielding to aero-space craft. The second goal is to provide thermal protection in hypersonic transport and entry into a planet's atmosphere. Finally, the third goal is to convert the thermal energy in electric energy. Many hurdles are left to overcome many of which would be impossible with the resources provide by LONI.

Presentations of the research:

S. Baker, "Molecular modeling scheme to efficiently determine the selectivity of various calix-crown molecules with Cs, K, and Na ions." S. Baker, B. Ramachandran, P. Derosa, Louisiana Academy of Science Feb. 2010.

S. Baker, "Molecular modeling scheme to efficiently determine the selectivity of various calix-crown molecules with Cs, K, and Na ions." S. Baker, B. Ramachandran, P. Derosa, Tera Grid 10 August. 2010.

Achievements:

Best Graduate Paper Louisiana Academy of Science 2010.

Wei Huang, LSU

Research:

Riboswitch RNAs are emerging cis-regulatory elements in Bacteria that control the expression of downstream genes. These regulatory elements have many potential applications. First, they can be drug targets for novel antibiotics. This is because riboswitches are found to be widely distributed in bacterial genomic sequences and important in modulating the metabolic pathways. What's more, recent findings also suggest the existence of riboswitches in human, which can be potential therapeutic targets for some diseases. Secondly, we can make artificial riboswitches in response to certain ligands to serve as a regulatory element in artificial bacteria. One idea is to use a riboswitch that can sense a certain pollutant to control the mobility of the artificial bacteria, which is also equipped with enzyme to degrade the pollutant. Therefore, the artificial bacteria can be used to track down the pollutant and degrade it. Last but not least, these complicated 3D structure motif found in riboswitches can be adopted to create self-assemble scaffolds for nano-fabrication. To facilitate these applications, it is of importance to explore the dynamics behaviors of riboswitch RNAs and to understand the linking between ligand binding and conformational adaptability of riboswitches.

The computational studies I have done so far have suggested a mechanism of ligand assisted folding on the SAM-I riboswitch system, the results have been published last year on Nucleic Acids Research. This provides us the hypothesis for our on-going experiments. One is the ligation experiment, in which we change the positions of the ligation site, as suggested in our simulations, to probe the effects of S-adenosyl methionine (SAM) on the folding of the SAM-I riboswitch. The other experiment is to develop a florescence assay, with which we can monitor the effects of different ligands on the folding of the SAM-I riboswitch. This assay can facilitate the screening of small molecule library to identify potential hits for further drug design.

In parallel, the experimental part I am working on is to modeling the 3D structure of the "ON" state of the SAM-I riboswitch via NMR and X-ray crystallography. There is little information about this state in the literature. The preliminary results we gained from experiments are used as inputs for computation predictions. For example, the base pair information revealed in our NMR spectrum is used in the secondary structure prediction for the "ON" state of this RNA. Moreover, we will use the structure from our experimental studies for Replica-exchange Molecular Dynamics (REMD) simulations to unveil the whole free energy folding landscape of the SAM-I riboswitch.

Publications of the research:

1. Huang, W., Kim, J., Jha, S. and Aboul-ela, F. (2009) A mechanism for S-adenosyl methionine assisted formation of a riboswitch conformation: a small molecule with a strong arm. Nucleic Acids Res, 37, 6528-6539.

2. Kim, J., Huang, W., Maddineni, S., Aboul-ela, F., Jha, S. Exploring the RNA Folding Energy Landscape Using Scalable Distributed Cyberinfrastructure. Emerging Computational Methods for the Life Sciences Workshop, 2010.

Presentations of the research:

1. Huang, W., Aboul-ela, F., Kim, J., Jha, S. and Boyapati, V. (2009) Dynamics differences of SAM-I riboswitch aptamer between SAM bound and without SAM: insight into conformational rearrangement. FASEB J., 23, 842.841.

Use of LONI and HPC resources:

I mainly use LSU HPCs. I submit batch jobs to set up MD simulations on Tezpur. And I use philip/santaka to analysis my data and generate visualizations to present the results. I am also using LONI HPCs to test the methodology of adaptively using the small clusters, such as eric, oliver, poseidon, etc.

Collaborations:

Dr. Mobley at UNO has given me suggestions on doing some binding free energy calculations, for example, MM-PBSA calculation.

Salman Javaid, UNO

Research:

The research goals for during this semester and for the academic year will be focused on various are of research in the area of forensics. After comprehensive analysis of different malware detection and mitigations techniques, it was proposed that design and development of hardware-assisted introspection architecture is required for supporting advance introspection-based malware detection and mitigation strategies. Techniques for deep, portable modeling of kernel data structures via introspection are highly required because this will not only bridge the semantic gap between the physical memory provided by the introspection and the high-level kernel structures in a guest operating system hosted by the VMM (Virtual Machine Manager) but also be useful in addressing portability issues. Main area in this aspect is focused on the automated adaption of our tools to various types of kernels out there. Thus a strategy to adapt to various kernels under live forensics is being developed. Also techniques for real-time verification of critical kernel code and cross-verification of kernel structures are also being developed parallel to the previous project.

The parallelization of our tools is an essential part of our project. Together with GPU parallelization, we are considering using LONI facilities to conduct various parallel version of our tool and study the effect of parallelization of out tools in a distributed environment. This will show us that which environment is best for developing high grade and effective live forensics malware detection tools.

Pavel Klimovich, UNO

Research:

I am writing to inform you that during the year of my LI Graduate Fellowship I was involved in two major projects both of which required utilization of the LONI computational facilities. In my first project, I was predicting the hydration free energies of a set of small organic molecules that are claimed to be potential drugs which makes this sort of study be important for pharmaceutical companies and, in more general sense, for all drug designers regardless of whether they are experimental or computational chemists. Indeed, the results obtained from that work turned out to be in good agreement with existed experimental data which made it worth publishing in a peer-reviewed journal (Ref 1). Also, this work was presented (Ref. 2) at the UNO Chemistry Department poster session and was awarded first prize in the beginning graduate student category.

In my second project, I employed similar methodology to investigate the binding affinity of several benzamidinium derivatives to the protein trypsin. Trypsin, an important target for medicinal chemists, is known to be sensitive to lysine or arginine that are able to reduce its physiological activity. Thus, molecules or ions (e.g. benzamidinium ion) that mimic these amino acids are potential non-natural inhibitors of trypsin and are subject to intensive study.

Since binding affinity prediction is a more challenging task than computing the hydration free energy, it was not a surprise that first calculated affinities had a discrepancy with the experimental data. Nevertheless, analysis of these intermediate results provided us with a feeling on how the model should be modified to improve the computed values of the binding free energies. Because of the high interest to the trypsin shown, we anticipate publishing this work as well once completed.

Publications of the research:

1. Pavel V. Klimovich and David L. Mobley, "Predicting hydration free energies using all-atom molecular dynamics simulations and multiple starting conformations", J. Comp. Aided Mol. Design 24:307, 2010.

Presentations of the research:

2. Pavel V. Klimovich and David L. Mobley, "Computational prediction of small-molecule hydration free energies". First prize winner at the UNO Chemistry Department poster session, October 2, 2010.

Hongzhi Lan, Tulane

Research:

The three-dimensional (3-D) numerical simulation of cell motion and deformation in shear flow is carried out in this research. Cellular deformability may lead to lateral migration of cells toward the centerline during their perfusion in a microfluidic flow chamber. This property can be used for separation of cells of different deformabilities, such as, for example, red and white blood cells. We study the effect of bulk viscoelasticity on lateral migration of cells and particles in shear flow using custom computational fluid dynamics code. The cells and particles are modeled as multiphase (a nucleus surrounded by a layer of cytoplasm) and single-phase viscoelastic drops, respectively. The numerical algorithm is based on the volume-of-fluid continuous-surface-force (VOF-CSF) method and the semi-implicit solvers for the Navier-Stokes equations and the Giesekus constitutive equation for bulk viscoelasticity. Our simulations show the cell/particle with larger deformability moves at a lower translational velocity than the fluid flow. At the same time, it migrates with a relatively constant velocity toward the channel centerline until reaching the equilibrium position. A more deformable cell is characterized by a higher lateral migration velocity.

Publications of the research:

Not so far. I'm still doing simulation and data analysis.

Presentations of the research:

1. "Simulation of Cell Motion and Deformation in Shear Flow with MPI Parallel Programming" in 2010 Tulane SSE Research Day Poster Session on April 8th, 2010.

Use of LONI and HPC resources:

The research did much mathematical simulation by running computational code on multiple-processor nodes of CCS computer clusters.

Collaborations:

I had discussions with Dr. Khismatullin, Dr. Fujioka and Dr. Chrispell about the computational algorithms, data results and parallel programming.

Achievements:

I obtained the Honorable Mention award in Graduate Division of 2010 Tulane SSE Research Day Poster Session.

Kimberlee Lyles, SUBR

Research:

This past semester, I continued my research in molecular dynamics simulation of the gK and UL20 protein structures. Using a small portion of the gK protein structure, constructed by Dr.Shizhong Yang, I was able to analyze the structure visually and insert the protein inside of a 50 Å x 50 Å membrane. I was also able to create three script files that were required prior to the insertion. The script files included commands that calculated the center of mass of the protein, aligned the protein with relativity to the x, y, and z axis, combined the two structures together, and deleted lipid molecules from the membrane which overlapped the protein. During this time, I found that even this smaller structure can be extremely difficult to manipulate. I ran into countless problems during the process of writing the script files and attempting to align and combine the structures, as the alignment is very critical to the success or failure of the simulation. During the next month, I will continue to write another script file which contains the parameters necessary to run the molecular dynamics simulation. Since the final simulation is not complete as of yet, the results are yet to be determined.

Presentations of the research:

1. Dr. Shizhong Yang presented a poster in my absence at the Louisiana Academy of Sciences in February 2010.

Use of LONI and HPC resources:

I have used LONI and the HPC resources for test simulations.

Collaborations:

With SUBR faculty members

Achievements

I anticipate completing the full simulation of the gK fragment around mid-July 2010 and using the results in my defense for my thesis this July.

Narate Taerat, LA Tech

Research:

In order to come up with a good failure prediction for HPC system, we need to define what 'good' is. Under Dr. Chokchai (Box) Leangsuksun supervision, I derived two novel metrics measuring goodness of two major types of failure prediction: time-to-failure (TTF) prediction (regression type) and failure occurrence (FO) prediction (classification type). Instead of using balanced measurement like mean-squared error (MSE), we defined imbalanced metrics concerning the direction of predicted failure time relative to the actual time. We also discovered that traditional metrics (MSE, MAD, precision and recall) were sometimes misleading. Further details of these new measurements can be found in the publication listed below. In TTF prediction, most training methods use optimization (minimization) on prediction error measurement (e.g. MSE). Unfortunately, the metrics we derived are not continuous so we cannot just use the infamous critical point method. So, I am currently researching in piecewise convex optimization in order to apply the TTF metric to the training methods. In addition, I also participate in implementing the new HA-OSCAR, featuring OSCAR independence, automatic smart cloning, and stateful service backup plugin support.

Publications of the research:

1. IEEE ISPA 2010: Proficiency Metrics for Failure Prediction in High Performance Computing
2. IEEE ISPA 2010 (co-author): Benefits of Software Rejuvenation on HPC Systems

Use of LONI and HPC resources:

All of the productive systems in LONI could be beneficial to HPC reliability research if the reliability-related data (e.g. syslog) were obtainable.

Collaborations:

I cooperated with a LONI system administrator, Mr. Isaac Traxler, trying to obtain real syslog data from LONI production systems. Unfortunately, we could not resolve the issues about security and privacy, so the data were not accessible.

Shuxiang Yang, LSU

Research:

There are mainly three projects which I have been actively involved.

Firstly, we use quantum Monte Carlo simulation combining Maximum Entropy Method calculation and exact diagonalization to study the finite temperature dynamic structure factor of antiferromagnetic spin-1 chain and Zeeman e ect of its edge excitations. These results are compared with recent neutronscattering experiments and theoretical discussions on finite temperature dynamical properties of the system, and show a satisfactory agreement.

In a recent Letter (Phys. Rev. Lett. 103, 186403 (2009)) Efetov et al. propose an exact mapping of an interacting fermion system onto a new model that is supposed to allow sign-problem free Monte Carlo simulations. As the second project, we want to test this new idea. With our study (both theoretically and numerically), we find that their formalism is equivalent to the standard approach of Blackenbecker, Scalapino and Sugar (BSS) for fermionic systems and has the same sign statistics and minus sign problem.

Lastly we use the dynamical cluster approximation to understand the proximity of the superconducting dome to the quantum critical point in the two-dimensional Hubbard model. In a BCS formalism, the superconducting transition temperature may be enhanced through an increase in the d-wave pairing interaction (Vd) or bare pairing susceptibility (chi_0d). At optimal doping, where Vd is featureless, we find a power-law behavior of chi_0d(w=0), replacing the BCS logarithmic behavior, and a dramatic increase of low energy pair excitations. The well-known dome shape of superconducting phase diagram thus follows naturally. And we also suggest some experiments to verify our predictions.

Publications of the research:

1. "Comment on 'Exact bosonization for an interacting Fermi gas in arbitrary dimensions' ", accepted by Phys. Rev. Lett.

2. "Finite temperature dynamical properties of antiferromagnetic spin-1 chain ", to be submitted to Phys. Rev. B

3. "Proximity of the Superconducting Dome and the Quantum Critical Point in the Two-Dimensional Hubbard Model", to be submitted to Phys. Rev. Lett.

Presentations of the research:

"Numerical study of the bond order in 2D Hubbard model", talk, Portland, OR, APS March Meeting, 03/16/2010

Use of LONI and HPC resources:

I attended the computational physics course which is made available with the help of CCT.

And I also attended the Mardi Gras Conference 2010 hosted by CCT.

The availability of QueenBee super-computer is quite helpful to me when I debug our codes.

Collaborations:

We have some interaction with Dr. Abdelkader Baggag from Louisiana Tech University.

Linghang Ying, Tulane

Research:

The purpose of our project is to better understand the physics of rogue waves in deep water, and the probability of their occurrence as a function of environmental conditions (wind, current, wave speed, etc.) Oceanic rouge waves, or freak waves, are surface gravity waves whose wave heights are extremely large compared to the typical wave in a given sea state.

We use the current modified nonlinear Schrödinger equations (CNLS¬¬4) to construct a nonlinear model to simulate the ocean wave development, and obtain quantitative predictions of the wave height distribution as a function of the key parameters: average steepness, angular spread, and frequency spread of the incoming sea state. We find that for a wide range of parameters, a K-distribution (a convolution of Rayleigh and chi-square distributions, determined by a single parameter N) works well in describing the tail of the probability distribution. By obtaining N for each sea state, we can quantitatively predict the enhancement of freak wave occurrence probability at that sea state. Furthermore, we find simple power laws for the dependence of N on environment parameters for moderate values of the steepness. Thus we obtain a simple but quantitative model for the risk of rogue wave formation in a wide range of physically realistic sea conditions.

The long-term research goal is to study the interplay between nonlinear effects and wave-current interactions as well as finite-depth effects in coastal waters. Data on the rogue wave probability distribution as a function of current strength is currently being collected and analyzed.

Publications of the research:

The first manuscript "Systematic Study of Rogue Wave Probability Distributions in a Fourth-Order Nonlinear Schroedinger Equation" is being edited for publication, to be submitted this summer. A second manuscript on the interaction of nonlinear and current effects will be forthcoming

Presentations of the research:

A a poster in the annual Tulane science and engineering forum, on April 8 and April 18.

Use of LONI and HPC resources:

We use the louie cluster to run my MATLAB code that implements the CNLS¬¬4 equation and calculates rogue wave formation probabilities.