First Annual Report

LONI Institute PKSFI Project

June 30, 2007 – June 30, 2008

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Introduction

The LONI Institute (LI) was created to build a statewide collaborative computational science environment of faculty, staff, and students who will take advantage of the hardware investments made in LONI to advance research, education, and economic development in Louisiana.

The first year of the project has been primarily aimed at recruiting faculty, staff, and students for the project, and the milestones we list below reflect this. The PIs and Senior Investigators (SIs) have met in person, and had numerous conference calls, to coordinate their searches for graduate students, computational scientists, and faculty. In future years, the group will concentrate more on the research, education, and economic development activities outlined in its strategic plan.

In terms of hires to start up the Institute, in year 1 (Y1) we have supported 6 graduate students who have used LONI facilities to advance their research, hired the first 5 faculty (none of whom have started as of June, 2008), 4 computational scientists, and the scientific coordinator for the entire project (just hired May 30). Searches continue for the remaining faculty and computational scientists.

The existing LI faculty and staff (the PIs and SIs), the staff of LONI itself, and the staff of the Center for Computation & Technology have worked together on numerous projects and proposals, and have held outreach and training sessions across the state. The largest of these projects is the $12M NSF-EPSCOR RII project entitled CyberTools (see http://cybertools.loni.org), which was awarded in October 2007, involves most of the LI Institutions and many of its members, and aims to develop an advanced cyberinfrastructure for statewide research. As this project moves forward, and as LI personnel continue to be hired, CyberTools and the LI will become very tightly connected, and we expect many new projects to emerge from these. One can view these two projects as layered on top of the LONI infrastructure, with Cybertools focusing on software, services, and applications, and the LI focusing on collaborations and projects.

In summary, the project activities are ramping up and should accelerate in year 2 as the first wave of hires arrives, more projects begin, and more faculty, staff, and students are recruited.

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 an outline 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. Deliverables for Y1 are highlighted in yellow, while deliverables for "the end of year x", including Y1, are highlighted in green.

At the end of each item, we provide information collected for this first annual report. We highlight specific progress by institution where notable.

The LI is at its beginning stage, but we have collected data from people who are associated with LI to illustrate the kinds of activities we expect to be driven specifically by the LI as we get the new staff and faculty in place. In particular, we mention the CyberTools project, which even though it was applied for before the LI started, was funded after the LI started. The people who formed the LI built relationships while also planning and proposing the CyberTools project.

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.	5 fellows hired by the EOY1 (Sec. 1.I.a).
Development Coordinator	Individual hired	1 hire, Fall Y1; new hire in 6 months if position becomes vacant	Individual was hired. (Sec. 1.I.e).

LI Graduate assistantships	Graduate students funded by Institute	6 in each 2 year period; 18 students total over life of project	6 Graduates Fellows funded (Sec. 1.I.c).
LI Computational Scientist	Individual hired	6 hired in Fall Y1; new hire in 6 months if position becomes vacant	4 CSs hired (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	7 positions funded (Sec. 1.I.b).

1.I.a) Full-time faculty hires

Concerning the full-time faculty hires, our success criterion is the hire of 6 faculty members by the end of Y2. During Y1, five LONI Fellows were hired, with most of them having a start date in Y2. Institutions that have not filled their two LI Fellow positions continue their searches, review of applications, and interview process. Here is the list of the LONI Fellows by institution.

LSU: One professor has been hired: Dr. Mark Jarrell, Physics. His start date is January 2009. Dr. Jarrell's main area of interest lies in the physics of strongly correlated electronic materials, which include many nanostructures, high T_c superconductors, and heavy Fermion and magnetic materials.

LA Tech: Two professors have been hired: Dr. Abdelkader Baggag in Computer Science, and Dr. Dentcho Genov in Physics and Electrical Engineering. Their start date is September 2008. Dr. Baggag's main research is in the area of high-performance computing applied to engineering problems, in particular, developing innovative parallel numerical algorithms for large-scale industrial applications, and ensuring their efficient implementation of high-end computers. Dr. Genov's background spans different areas of research in Physics and Engineering. His major interests are in electromagnetic theory and its applications in a wide variety of systems, including nanoscale complex media, novel type of metamaterials, nano-, and mesoscopic particles and their optical properties, plasmonics and nanophotonics, nonlinear optical effects, and applications. He has extensive experience in modeling actual devices ranging from nano-sized optical elements, to large scale plasma focus discharge machinery. During the next five years, he intends to focus his research on studies of the fundamental nature of EM wave interaction with meso- and nano-structured metamaterials.

Tulane: One professor has been hired: Dr. Damir Khismatullin in Biomedical Engineering. He was hired in June of 2008 as an Associate Professor. He will join the department and the CCS on August 1, 2008. Dr. Khismatullin's research is connected to computational fluid mechanics and cell-tissue engineering, and his interests include computational and theoretical studies of receptor-mediated leukocyte adhesion to endothelium. More

generally, he has expertise in cellular biomechanics, biophysics, bio-fluid mechanics, medical ultrasound, multiphase and non-Newtonian flow. In addition to his duties in the BME department, Dr. Khismatullin will be an active participant at the CCS and is expected to initiate new computational projects, teach computation courses, and supervise multidisciplinary students.

UNO: One professor has been hired: Dr. David Mobley, Chemistry. His research is in Medicinal Chemistry, and his start date is July 2008.

1.I.b) Federal funding for additional staff

The LI encourages submission of proposals that add federally-funded staff to LONI. We have 7 staff positions currently funded by the LONI HPCOPS project from NSF. We refer you to http://www.hpc.lsu.edu//about/ (the positions that say TeraGrid at the end are HPCOPS-funded).

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

Below, we show a list of the Y1 LI Graduate Student Fellows. We also provide a brief description of the research they have done.

Graduate Fellow	**Institution**	**Field**
Jijun Lao	LSU	Mechanical Engineering
Phani Dathara	LATECH	Engineering (Micro/Nano-Technology)
Frank DeTiege	SUBR	Mechanical Engineering
Xiaolan Zhou	Tulane	Physics
Jin-Feng Chen	ULL	Computer Science
Huy Pham	UNO	Physics

-- Jijun Lao (LI Graduate Fellow from LSU for 2007-08)

During the last year he studied the novel structural instability and shape memory effect in metallic nanowires using molecular dynamics simulations on the massively parallel computers of LONI Institute. In this study, he investigated the fundamentals of surface-stress-induced phase transformation and pseudoelastic deformation processes in palladium nanowires using molecular dynamics (MD) simulation.

The results of his research were presented in the proceeding of TMS 2008 Annual Meeting and recently were submitted to the journal of Applied Physics Letters (currently under review). His immediate goals are to continue to utilize the high performance computing resources from LONI Institute and to expand his research expertise in the area of modeling and simulation of nanostructured materials.

Publications

1. Jijun Lao, Dorel Moldovan. "Surface stress induced phase transformation and pseudoelastic effect in palladium nanowires". *Applied Physics Letters*, submitted 2008

2. Jijun Lao, Dorel Moldovan. "Surface stress-induced structural reorientation and shape memory effect in Pd nanowires". *TMS 2008 Annual Meeting Proceeding*, Hael Mughrabi Honorary Symposium: Plasticity, Failure and Fatigue in Structural Materials - from Macro to Nano, March 10, 2008

-- Gopi Krishna Phani Dathara (LI Graduate Fellow from LA Tech for 2007-08)

In his dissertation research, investigating complex metal hydrides as potential materials for solid state hydrogen storage, he employs computational chemistry tools to model and analyze the nanomaterials which require high performance computing facilities. Financial assistance provided through graduate fellowship from LONI and computational resources provided by LONI through IBM p-5 clusters have been very helpful in the advancement and great progress of his research. Continuing research in this area resulted in one invited paper accepted for publication in a peer reviewed journal, one paper in conference proceedings, two oral presentations at the AIChE national conference annual meetings and an oral presentation at AIChE spring national meeting:

1. G.K.P. Dathara and Mainardi D.S., Structure and Dynamics of Ti-Al-H Compounds in Ti-Doped NaAlH4, Molecular Simulation, 34(2), 201-210, (2008)

2. Phani Dathara G. K. and Daniela S. Mainardi, Modeling Effects of Titanium Dopants on Hydrogen Adsorption/Desorption kinetics by Sodium Alanates, AIChE Annual Meeting Conference proceedings, Nov 4 ? 9, 2007, Salt Lake City, Utah.

3. Phani G. K. Dathara and Daniela S. Mainardi, Structural, Energetic and Thermodynamic Studies of Acrylic (PAA, PMA and PMMA) and Allylamine (PAH) Polymers for Self Assembly, AIChE Spring National Meeting, April 22 -26, 2007, Houston, TX.

4. Phani G. K. Dathara and Daniela S. Mainardi, Dopant and Vacancy Effects on Hydrogen Adsorption/Desorption by Aluminum-Based Complex Hydrides, AIChE annual National Meeting, Nov 12-17, 2006, San Francisco, CA

-- Frank DeTiege (LI Graduate Fellow from SUBR for 2007-08)

His research encompassed the study of enhancing heat transfer in pressurized water reactors. The goal of this research was to determine if heat transfer can be enhanced by modifying plain surfaces with extended surfaces. Fluent, CFD, software was used to simulate the heat transfer from the extended surfaces' models.

-- Xiaolan Zhou (LI Graduate Fellow from Tulane for 2007-08)

Xiaolan works with Prof. John Perdew on computing the formation of energy of an atomic vacancy in metals (aluminum) and semiconductors (silicon) using standard density functional approximations as well as new density functional developed by their group. The goal was to improve results using the new approximations compared with experimental values and shed new light on properties of materials. The computations using DFT often need to include a large number of atoms and are extremely intensive. For this, the LONI systems have been indispensable. One of the difficulties is that experimental values contain errors and their exact accuracy is unknown. The energies computed by the new approach include surface energy and curvature energy. This research project is on-going.

Xiaolan Zhou gave a presentation on this work at the March meeting of the American Physical Society in New Orleans in 2008. She also presented posters with preliminary results at the Tulane University Research Day in April of 2008 and the Engineering Forum at Tulane in May of 2008.

-- Jin-Feng Chen (LI Graduate Fellow from ULL for 2007-08)

The objective of his proposed work was to develop a methodology of constructing 3D models that can be used as engineering analysis tools for highway infrastructure systems. His plan was to analyze the image and video data collected from a driver's perspective and to extract information pertinent to the roadway, including the road surface, the shoulder areas, guardrails, traffic control devices, and all roadside elements. The information will be integrated into a 3D environment that will give engineers new tools to examine and identify highway features such as the degree of curvature, superelevation, sight distance, and pavement edge lines. This tool will enable highway engineers to design and evaluate highway infrastructures from new perspectives, which are not feasible with the currently available technologies. The specific technical objectives for the first year were:

1. Identify the road lanes and the shoulder area from the video data;

2. Map the identified image features into a 3D model;

3. Render the 3D road model as a virtual reality playback on a workstation, such as through a Web browser plug-in.

-- Huy Pham (LI Graduate Fellow from UNO for 2007-08)

His research interests mainly concern theoretical work in the domain of simulation of magnetization dynamics in nanostructured materials. The dynamic switching behavior of magnetization was investigated based on the Landau-Lifschitz-Gilbert equation and Stoner-Wohlfarth model. The main goal of the study was to reduce the switching time of magnetization as well as to increase the recording density of the magnetoresistive random access memories (MRAM) and other data storage devices. Current interest is investigating the influence of spin transfer torque on switching behavior of magnetization.

Papers:

Switching behavior of a Stoner-Wohlfarth particle subjected to spin-torque effect, H. Pham, D. Cimpoesu, A. Stancu, and L. Spinu, J. Appl. Phys. 103(7), 07B105-1-3 (2008), http://dx.doi.org/10.1063/1.2830720

Presentations:

1. Dynamic and temperature effects in spin-transfer switching, H. Pham, D. Cimpoesu, A. Stancu, and L. Spinu, Intermag 2008 Conference, May 4-8, 2008, Madrid, Spain, paper CN-01, pp. 419 - poster presentation
2. Dynamic and temperature effects in spin-transfer switching, D. Cimpoesu, H. Pham, A. Stancu, and L. Spinu, 2008 American Physical Society (APS) March Meeting, March 10-14, New Orleans, Louisiana, paper A15.00006 - oral presentation, http://meetings.aps.org/Meeting/MAR08/Event/74841
3. Switching behavior of a Stoner-Wohlfarth particle subjected to spin-torque effect, H. Pham, D. Cimpoesu, A. Stancu, and L. Spinu, 2008 American Physical Society (APS) March Meeting, March 10-14, New Orleans, Louisiana, paper D32.00001 - oral presentation, http://meetings.aps.org/Meeting/MAR08/Event/76356

1.I.d) LI Computational Scientists:

A crucial component of the LI is a strong contingent of advanced staff computational scientists. 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 Katz).

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.

Here are the CSs the LI has hired so far.

SUBR: Dr. Shizhong Yang. He started on May 2008. He obtained his Ph. D. in Computational Physics with a co-discipline in Electrical Engineering from the University of Missouri-Kansas City, in 2006.

Tulane: Dr. Hideki Fujioka, whose first day of work at CCS was Friday June 20, 2008. He is going to be housed at the Center for Computational Science at Tulane. Dr. Fujioka has a B.S. degree in Mechanical Engineering, an M.S. degree in Biomedical Engineering and a Ph.D. in Biomedical Engineering. For the last 10 years, Dr. Fujioka has been a Postdoctoral researcher at Imperial College of London, and a researcher in the BME department at the University of Michigan in Ann Arbor. His expertise is in computationally efficient simulations of fluids in channels in a variety of settings including surfactants, pulsatile blood flows, mass transport, and gas transport. Dr. Fujioka has substantial experience developing complex codes (e.g. CFD) in serial and parallel platforms using MPI as well as developing tools to analyze data such as CT-images. At the CCS, his primary focus will be to improve the overall efficiency of the work done on all projects by increasing computational speed, parallelizing codes that are currently serial, working with postdoctoral and senior researchers on improved programming and post-processing practices.

ULL: Dr. N. Raju Gottumukkala started on January 10, 2008. Dr. Gottumukkala graduated with a Ph.D. from Louisiana Tech in the area of High Performance Computing, with a strong background in Computational Science and Discrete Mathematics

UNO: Zhiyu Zhao received her B.E. (1997) and M.E. (2000) degrees in Computer Engineering from the Huazhong University of Science and Technology, China. In the year 2004 with a governmental scholarship she initialized her Bioinformatics research in DNA micro-array data analysis at the Politecnico di Milano University, Italy. In the year 2005 she started her study in the Department of Computer Science at the University of New Orleans. She received a M.S. degree in Computer Science in 2006. Currently she is a Ph.D. candidate expecting summer 2008 graduation. Her research field is Bioinformatics and her current research topics include protein 3-D structure alignment, protein structure searching from the Protein Data Bank, haplotype reconstruction from SNP matrices with incomplete and inconsistent errors, and genome comparison based on non-breaking similarity.

1.I.e) LI Scientific/Development Coordinator:

The LI recently hired Dr. Bety Rodriguez-Milla as the scientific coordinator. Her start date was May 30, 2008. She will assist in coordinating LI activities, including grant development, educational programs, assessment of applications for students and associated faculty, tracking projects and milestones, organizing workshops, training sessions, coordinating HD courses, etc.

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	24 projects using LONI (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	491 users, 119 of them have logged on in the past 6 months (Sec. 1.II.c).
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	N/A
Research computing project resources	Successful computational infrastructure/cycle applications	50% of projects lead to nationally-judged computational infrastructure awards in Y2 and subsequent years	N/A
Research publicity	Invited presentations and lectures outside LA	Each project leads to 2 presentations/lectures per year starting in Y2; 160 total	N/A
Scientific &	Peer-reviewed conference and journal	3 per LONI Fellow per year; 1 per LI project per	Numerous acknowledging

Engineering Results	publications that acknowledge LI support	year; over 150 total	LONI (Sec. 1.II.b).
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	N/A

1.II.a) LI Projects underway

Here we list the projects by institution.

LA Tech:

Neven Simicevic (neven@latech.edu)

1. Bioeffects of non-ionizing UWB radiation, sponsored by Air Force Office of Scientific Research
2. Underground imaging, sponsored by JD (I would not mention the company)
3. Underground imaging, sponsored by Gas Technology Institute (GTI)

Daniela Mainardi (mainardi@latech.edu)

1. DoE BES DE-FG02-05ER46246 "Understanding the local atomic level effect of dopants in complex metal hydrides using synchroton x-ray adsorption spectroscopy and density functional theory."
2. NSF-CTS-0449046 "CAREER: Modified-Methanol Dehydrogenase Enzymatic Catalysts For Fuel Cell Devices."
3. BoR-Enhancement LEQSF(2007-08)-ENH-TR-46 "Computer Laboratory Enhancement for Nanotechnology Education."

Bala Ramachandran (ramu@latech.edu)

1. Correlation Energy in Density Functional Theory Funcionals
2. Computational Modeling of Organolithium Chemistry

3. Acidities of Aromatic Hydrocarbons in Aqueous Solutions under Normal and Supercritical Conditions

4. *International Chemistry Research Experiences for Students in Vietnam*, National Science Foundation (OISE – Global Scientists & Engineers), L. M. Pratt (PI), Allan R. Pinhas (Co-PI), $150,000. [OISE-0744375]

Collin Wick (cwick@latech.edu)

1. Computational Modeling and Design of Polymer Electrolytes for Lithium-ion Batteries, LA BoR (RCS), $118,555.

SUBR:

Dr. Shizhong Yang is working on two projects now:

1. Thermo-barrier coating project. Thermal barrier coatings (TBCs) are used in the hot section of rocket engines and jet engines to safeguard the engines under extreme working temperature, ~1600ºC. In this project, Southern researcher, Dr. Yang and group members is doing computer simulation on ZrO2/Al2O3 interface, while Dr. Shengming Guo's research group at LSU is doing plasma spray experiment in collaborate with NASA scientists. This project was funded by NASA EPSCoR–BoR for one year with total budget $61125.00 /yr (Southern was allotted $22250.00);
2. gK and UL20 secondary structure prediction in Herpes Simplex Virus Type 1. Understanding the secondary structures of gK and UL20 could greatly facilitate predicting functional domains of each protein that may be involved in multiple functions through the virus lifecycle. In this project, Dr. Shuju Bai, Dr. Shizhong Yang and the graduate students are collaborating with Dr. K. G. Kousoulas group at LSU Veterinary Medicine, using related computational tools to predict second order protein structures of gK and UL20. This is a one year $50000.00 /yr LBRN fund-pending project. Dr. Bai is the principal investigator and Dr. E. Khosravi, Dr. M. Newcomer and Dr. Kousoulas are the mentors. An undergraduate student, Kiara Williams, who was supported by Southern HBCU-UP SMART program, is working with Dr. Yang on this project. She will make a presentation at the end of this Summer semester.]

Tulane: The Tulane faculty named as Principal or Senior Investigators in the LONI Institute carry out this research at the Center for Computational Science. Associated projects are:

1. During the 2007-08 academic year, Tulane hired Dr. Courtney Lopreore with a 30% appointment in the BME department and 70% in the CCS. During this time, Dr. Lopreore has worked on computational neuroscience. Specifically, she has developed a computational model for the electrodiffusion of ions in nerve fibers. The system studied consists of a neuronal axon and a glial cell and the goal is to determine the functional role of potassium channels and their relation to anatomical structure. Perform electrodiffusion simulations of ions will help understand how microscopic variations in anatomical structure affect potassium channel functioning and their contribution to signal transmission. The computational model involves

solving couples partial differential equations with discontinuous coefficients, generating complex computational meshes, and reconstructing tissue samples on the computer. Dr. Lopreore has started collaborations with Dr. Cortez on the computational issues and with Dr. Jeff Tasker (Cell and Molecular Biology department).

2. Computational and Experimental studies of the transmission of West Nile virus began in 2008 as a collaboration between the CCS and the department of Epidemiology at Tulane University. This seed project has been started thanks to internal funding at Tulane that includes funds for a postdoctoral researcher, laboratory staff, student trainees and laboratory supplies. Dr. Ivo Foppa (Epidemiology department, School of Public Health and Tropical Medicine) and Dr. Cortez are leading the project and are in the process of hiring the postdoctoral researcher. During the summer of 2008, Dr. Cortez has initiated a summer research program for undergraduate students, which includes a project in computational epidemiology to begin exploring appropriate models to use.

3. Beginning in 2007, CCS has led an NSF funded, focused research group that is developing analytical, computational and experimental tools to investigate the dynamics of elastic structures coupled to a complex fluid. Mucus transport by cilia in the respiratory tract, sperm penetration of the oocyte in fertilization, and peristaltic contractions of the oviduct are examples of such systems. Drs. Fauci and Cortez lead this effort, and beginning in August, a postdoctoral researcher (Dr. John Chrispell) and a graduate student (Ms. Sarah Lukens) will be at the CCS full-time as part of this research group. This focused research group is a collaboration with investigators from the University of California- Los Angeles, New York University, and Washington State University.

4. As part of a separate EPSCoR grant that includes several of the same universities of the PKSFI project, the PKSFI funds intellectual infrastructure that is being utilized by the EPSCoR project. The latter includes the development of an antibody-based biosensor. This is being approached from theoretical, computational and experimental angles in collaboration with investigators from Tulane, University of New Orleans, Xavier University and LaTech. The computational scientist hired at Tulane will help develop the computational tools required for the EPSCoR project. This type of synergy is quite important to our success in both projects.

5. A new project between Dr. Gaver and Dr. David Halpern (University of Alabama) is the computational investigation of physicochemical and fluid-structure interactions that occur during pulmonary airway reopening. This project involves the investigation of surfactant transport during the reopening of collapsed pulmonary airways, an understanding of which is critical to the development of advanced treatments of acute respiratory distress syndrome. In this project, we computationally model surfactant transport in the occlusion fluid and surfactant uptake to the air-liquid interface as a finger of air propagates through a flexible airway. This reopening process exposes the epithelial cells at the airway wall to large mechanical stresses, the magnitudes of which are predicted by computational

simulation. These simulations are performed using a combined boundary element method and volume of fluid approach. The computational facilities available through the LONI are instrumental to the success of this project.

6. Density functional theory is the most widely-used computational electronic structure method to predict what atoms, molecules and solids can exist, and with what properties. Until recently, improvements in the basic approximation for the exchange-correlation energy (coming partly from Tulane) have revolutionized quantum chemistry, but for condensed matter physics/materials science the local density approximation from 1965 has been almost accurate enough, and the new functionals that improved chemistry have helped little if at all. Professor John Perdew is trying to change that situation by restoring the density gradient expansion for exchange over a wide range of densities, with significant improvements to the lattice constants and surface energies of solids. He and his students and postdocs are beginning a series of tests and applications for real materials, including defects. Perdew and his group are now unofficial developers of the VASP and BAND codes for solids, which are being installed for them on CCS by Dr. Hideaki Kikuchi. The Tulane Physics Department hopes to hire a computational density functional theorist who might work with Dr. Perdew and with surface-science experimentalist Professor Ulrike Diebold

ULL:

The NIMSAT Institute at UL Lafayette has been leading the following projects, using the resources of LONI as well as the LONI Computational Scientist.

1. A Point of Distribution (POD) Tool for Commodities in Hurracane Affected Areas. Points-of-Distribution (PODs) are locations where in-kind donations of food, water, and other supplies received from the resource staging centers will be given directly to residents. Distribution points may be located in parking lots or open fields in the disaster area, as close to victims as possible. Setting up a POD is a complex problem involving several social, political and technological challenges. The NIMSAT Institute is developing an interactive POD planning tool for emergency managers to be able to geospatially analyze the post-disaster ground reality in terms of identifying the requirements of the victims, identifying the road-networks that are available so people can travel, available government facilities for setting up a POD, etc. Because of the computational complexity of the algorithm, and the need for immediate results post-disaster, the POD tool has been designed would to utilize computing resources of LONI on the back-end while providing an interactive web-based interface for the emergency management authorities to be able to use this POD planning tool.
2. An On-Demand Computing Framework for Disaster Management. Homeland security applications have to rely on massive volumes of data arriving from potentially hundreds and thousands of information sources that need to be computed, visualized and analyzed in real-time. “Urgent computing” is a new and evolving field made possible by the improved fidelity and utility of high-performance computing (HPC) to decision making. First responders, policy makers,

scientists and data analysts have to be able to collaborate via high-quality HD video sessions, share terabytes of data obtained from heterogeneous sources, perform interactive simulations and remotely visualize structured and unstructured data. Emergency managers, policy makers and first responders would need urgent access to super computing resources (computing systems, data storage systems, advanced instruments, data repositories, visualization environments) for disaster management. The NIMSAT Institute is developing a grid-portal based interface/framework for supporting end-to-end urgent computing for emergency management applications. This framework would consist of various tools to provision networks and data sources, provides urgent access to a workflow of applications created by multiple users, manage multiple urgent access requests and provide Quality of Service (QOS) guarantee for the users.

3. Advance resource reservation for interactive visualization jobs. Researchers at UL Lafayette and LITE are developing a VR-FlowVis framework as a part of the Cybertools project WP3, in partnership with LSU and other LONI institutions. This integrated VR-FlowVis framework would support interactive heterogeneous visualization environments by interconnecting various visualization tools for distributed data retrieval, parallelization frameworks in virtual environments (Viracocha), virtual reality toolkits (Vista) and application development environments (VRJuggler). All these tools would essentially be interconnected via the LONI network. Dr. Gottumukkala has begun working with Dr. Carolina Cruz-Neira and other LONI Institute researchers at UL Lafayette/LITE to provide an advanced resource reservation system for interactive visualization applications that would be a part of the VR-VFlowVis project.

UNO:

1. LONI Graduate Student, Pham Huy, under the direction of Dr. Leonard Spinu, works on micromagnetic simulations and uses the LONI supercomputers.
2. Brownian Dynamics simulation of binding of substrates to deep cavity cavitands. This project is being carried out by Dr. Scott Whittenburg.

1.II.b) Publications and Conferences Acknowledging LI support

The following are peer-reviewed conference or journal publications that acknowledge LI or LONI support.

LA Tech:

Papers:

1. Simicevic N. Exposure of biological material to ultra-wideband electromagnetic pulses: dosimetric implications. Health Physics. The Radiation Safety Journal. 92(6):574-583, 2007.

2. Simicevic N. FDTD computation of human eye exposure to ultra-wideband electromagnetic pulses. Phys. Med. Biol. 53: 1795-1809; 2008.

3. Ghouri M. M., Yareeda L., Mainardi D. S. "Geometry and Stability of Be_nC_m (n=1-10; m=1,2,…to 11-n) Clusters", *J. Phys. Chem. A*., 111(50), 13133-13147 (**2007**). http://pubs.acs.org/cgi-bin/article.cgi/jpcafh/2007/111/i50/pdf/jp075931c.pdf

4. G.K.P. Dathara and Mainardi D.S., "Structure and Dynamics of Ti-Al-H Compounds in Ti-Doped $NaAlH_4$", *Molecular Simulation*, 34(2), 201-210, (**2008**).

5. N.B. Idupulapati and D.S. Mainardi, "A DMOL3 Study of the Methanol Addition-Elimination Oxidation Mechanism by Methanol Dehydrogenase Enzyme", *Molecular Simulation*, In Press.

6. L. Pasumansky, C. J. Collins, L. M. Pratt, N.V. Nguỹên, B. Ramachandran, and B. Singaram, "Solvent and temperature effects on the reduction and amination reactions of electrophiles by lithium dialkylaminoborohydrides," J. Org. Chem. 72, 971-976 (2007).

7. M. M. Ghouri, S. Singh, and B. Ramachandran, "Scaled Density Functional Theory Correlation Functionals," J. Phys. Chem. A. (Robert E. Wyatt Festschrift) 111, 10390-10399 (2007). [Among the top 20 most-downloaded papers for third quarter of 2007.]

8. 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," J. Org. Chem. (submitted).

9. C. D. Wick and L. X. Dang, "Molecular Dynamics Study of Ion Transfer And Distribution at the Interface of Water and 1,2-Dichloroethane," Journal of Physical Chemistry C 112 (2008) 647-649. Cover article.

10. C. D. Wick and L. X. Dang, "Recent Advances in Understanding the Transfer of Polarizable Ions Across Aqueous Interfaces," Chemical Physics Letters 458 (2008) 1. Invited Review, Cover article.

Conference:

1. N. Simicevic, International Workshop on EMF Dosimetry and Biophysical Aspects Relevant to Setting Exposure Guidelines, 20 - 22 March 2006, Berlin, Germany.

2. N. Simicevic, 2008 Asia-Pacific Symposium on Electromagnetic Compatibility in conjunction with the 19th Intern. Zurich Symposium on Electromagnetic Compatibility, May 19 - 22, 2008 Singapore.

3. Veeramallu R., Kunjamon A. and Mainardi D.S., "CO_2 Conversion to Methanol and Ammonia Activation of Methanol Dehydrogenase Enzyme upon Methanol Binding", Proceeding paper of the National conference of the American Institute of Chemical Engineers (AIChE), Salt Lake City, UT, Nov 4-9, **2007**.

4. Idupulapati N.B. and Mainardi D.S., "Methanol Electro-Oxidation By Ion-Modified Methanol Dehydrogenase Enzymes", Proceeding paper of the National conference of the American Institute of Chemical Engineers (AIChE), Salt Lake City, UT, Nov 4-9, **2007**.

5. Keeton K.L and Mainardi D. S. "Characterization Of Mediators Proposed To Better Facilitate Electron Transfer In Methanol Dehydrogenase Enzymatic Fuel Cells", Proceeding paper of the National conference of the American Institute of Chemical Engineers (AIChE), Salt Lake City, UT, Nov 4-9, **2007**.

6. Keeton K.L and Mainardi D. S. "Nano/bio-Systems Modeling In Undergraduate and Graduate Education Using Gaussian '03 and Material Studio", Proceeding paper of the National conference of the American Institute of Chemical Engineers (AIChE), Salt Lake City, UT, Nov 4-9, **2007**.

7. Dathara P.G.K and Mainardi D. S. "Modeling Effects of Titanium Dopants on Hydrogen Adsorption/Desorption Kinetics by Sodium Alanates", Proceeding paper of the National conference of the American Institute of Chemical Engineers (AIChE), Salt Lake City, UT, Nov 4-9, **2007**.

8. Ghouri M. M. and Mainardi D. S. "Carbon Based Lithium Metal Hydrides for Hydrogen Storage", Proceeding paper of the National conference of the American Institute of Chemical Engineers (AIChE), Salt Lake City, UT, Nov 4-9, **2007**.

9. "Calculations of the acidities of n-butylbenzene protons in aqueous media under normal and supercritical conditions," P. Alburquerque, T. Junk, and B. Ramachandran, poster preseted at the 2008 ACS National Meeting, New Orleans, April 5-8, 2008.

LSU:

1. Michael Koppitz, Denis Pollney, Christian Reisswig, Luciano Rezzolla, Jonathan Thornburg, Peter Diener, and Erik Schnetter. Recoil velocities from equal-mass binary-black-hole mergers. Phys. Rev. Lett., 99:041102, 2007. (doi:10.1103/PhysRevLett.99.041102)
2. Jonathan Thornburg, Peter Diener, Denis Pollney, Luciano Rezzolla, Erik Schnetter, Edward Seidel, and Ryoji Takahashi. Are moving punctures equivalent to moving black holes?. Class. Quantum Grav., 24:3911–3918, 2007. (doi:10.1088/0264-9381/24/15/009)
3. David Brown, Olivier Sarbach, Erik Schnetter, Manuel Tiglio, Peter Diener, Ian Hawke, and Denis Pollney. Excision without excision. Phys. Rev. D, 76:081503(R), 2007. (doi:10.1103/PhysRevD.76.081503)
4. Luciano Rezzolla, Peter Diener, Ernst Nils Dorband, Denis Pollney, Christian Reisswig, Erik Schnetter, and Jennifer Seiler. The final spin from the coalescence of aligned-spin black-hole binaries. Astrophys. J. Lett., 674:L29–L32, 2008. (doi:10.1086/528935)

5. Burkhard Zink, Erik Schnetter, and Manuel Tiglio. Multi-patch methods in general relativistic astrophysics – I. Hydrodynamical flows on fixed backgrounds. Phys. Rev. D, 77:103015, 2008. (doi:10.1103/PhysRevD.77.103015)
6. Erik Schnetter, Christian D. Ott, Peter Diener, and Christian Reisswig. Astrophysical applications of numerical relativity — from Teragrid to Petascale. The 3rd annual TeraGrid Conference, TeraGrid '08 (accepted), 2008.

Tulane:

Published papers:

1. Smith, B.J. and D. P. Gaver III, The pulsatile propagation of a finger of air through a fluid-occluded cylindrical tube. *J. Fluid Mech.,* **601**: 1-23, 2008.
2. Perdew, J.P., Ruzsinszky, A., Csonka, G.I., Vydrov, O.A., Scuseria, G.E., Constantin, L.A., Zhou, X., and Burke, K., Restoring the density gradient expansion for exchange in solids and surfaces, *Phys. Rev. Lett.* **100**, 136406 (2008).

Presentations:

1. Pillert, J.E. and D.P. Gaver III. The experimental evaluation of asymmetric ventilation waveforms. Annual Meeting of the Biomedical Engineering Society. Los Angeles, CA. October, 2007.
2. J.P. Perdew, Simple density functional for solids and surfaces, John van Guens Lecture, 12th International Conference on the Applications of Density Functional Theory in Physics and Chemistry, Amsterdam, August 2007.

1.II.c) LONI USERS:

Currently, there are 491 Louisiana users with LONI accounts, of whom 119 have logged on to a LONI system in the past 6 months.

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	Program established	15 students at community college trained in CS each year, 30 total placed in	None

Competitiveness		companies, 10 enter universities for continued study in CS	
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	1 in progress (Sec. 1.III.c).
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)	One submitted proposal (Sec. 1.III.d).
New companies formed	Number of new companies	1 by EOY3, 3 by EOY4, 6 by EOY5	Two from staff and faculty related to the LI (Sec. 1.III.e).

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.

From LSU, there is a number of students from CCT working at Labs this summer; Farid Harhad (Schlumberger), Tyler Barker, Ian Wesley Smith (Microsoft).

From LA Tech, we refer you to Simicevic's projects 2 and 3. We cannot reveal the company's name on Project 2 because of a confidentiality agreement.

From ULL, two students of the NIMSAT Institute, Marc A. Reviere and Blaze Stutes, have been offered a summer internship with one of their private sector partners, the James Lee Witt Associates.

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

LSU is building towards joint projects with Schlumberger. LSU put in a joint proposal with Dell for Track 2C, a $30 million NSF call for national supercomputing resources. LSU also has a research partnership with NVIDIA.

At ULL, the following are the partner sector partners of the NIMSAT institute. These partners are all candidates for the use of LONI Institute's technical and intellectual assets, through their association with the NIMSAT Institute.

Partner Institution	***State***
AidMatrix/American Logistics Aid Network	*Texas*
Baron Services	*Alabama*
CISCO, Inc.	*California*
CommandNet Technologies	*Louisiana*
Fritz Institute	*California*
Genesys	*California*
Global eSolutions Group	*North Carolina*
IBM	*California*
IntraPoint	*Washington, DC*
James Lee Witt Associates	*Washington, DC*
*Lockheed Martin**	*Maryland*
MIEMAR Institute	*Louisiana*
Priority 5	*Massachusetts*
Rextag Strategies	*California*
SGI, Inc.	*California*
Wal-Mart Corporation	*Arkansas*

1.III.c) Sponsored Research with Companies

UL Lafayette Center for Business and Information Technologies, home of the LONI Institute, is working on a geo-physical visualization application called AMIGO™ in partnership with Fusion Technologies, Houston, TX. AMIGO is an application for visualizing and manipulating sub-surface geo-physical measurement data. For the oil and gas industry, this application would provide faster, easier and more unique views of the data enabling innovative approaches for oil and gas exploration.

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

Built on the foundations of the National Incident Management Systems and Advanced Technologies Homeland Security (NIMSAT) Institute, the University of Louisiana at Lafayette, Louisiana State University and their national partners (Team NIMSAT) has submitted a proposal for the establishment of the NIMSAT National Center of Excellence (COE) for Command, Control, and Interoperability for the DHS. The proposed COE would leverage homeland security institutes with existing missions, management teams, R&D infrastructure, and national scale partnerships to support the DHS mission. Furthermore, the COE will also capitalize upon more than $200M of IT investments into cyberinfrastructure and a strategic Gulf Coast location (a natural laboratory for all-hazards research and validation) to support the DHS mission. The COE will conduct research, develop tools, and provide education, training, and operational support to enhance national security.

The main goal of the COE is to create a suite of tools that empower analysts, first responders, and decision makers in rapidly analyzing data to deter, prevent, prepare, respond to and recover from all-hazards. Team NIMSAT seeks to enhance the ability of the DHS to manage security threats in an urgent and timely manner to safeguard lives, the economy, and critical infrastructures, leveraging advanced technologies such as high-performance computing, knowledge management, and visualization. The COE will advance the current scientific frontiers and state-of-the-art/practice in homeland security through a national public-private consortium.

1.III.e) Progress in Forming New Companies Related to Faculty, Staff or Students

A new faculty start-up company called Ultrascan includes one faculty member at LaTech, Dr. Erez Allouche. The company is developing a product that relies heavily upon a technology that Dr. Allouche is developing (there is a license agreement between LaTech and Ultrascan). This technology is highly dependent upon modeling and simulation.

The company Biofluidica Microtechnologies is run by David Claypool, Yohannes Desta, Steven A. Soper, who are staff and faculty working at LSU. BioFluidica Microtechnologies is a developer of unique compact/portable instruments capable of automated, fast, low-cost, point-of-use DNA tests for applications in human identification (forensics, paternity), medical diagnostics, and pathogen detection (food/water safety and biosecurity).

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.IV.a).
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.IV.a).
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.IV.b)
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.c).

1.IV.a) Interdisciplinary Papers, Conferences and Technical Reports

These interdisciplinary papers, conferences and technical reports can be cross-institution, and some of them are at the interface between biology, materials, and computational science. Here is the list of those by institution.

LSU:

1. Bogden, P. S., T. Gale, G. Allen, J. MacLaren, G. Almes, G. Creager, J. Bintz, L. D. Wright, H. Graber, N. Williams, S. Graves, H. Conover, K. Galluppi, R. Luettich, W. Perrie, B. Toulany, Y. P. Sheng, J. R. Davis, H. Wang, D. Forrest, Architecture of a community infrastructure for predicting and analyzing coastal inundation, Marine Technology Society Journal, 41, No 1: 53-71, 2007.

2. Yun, Z., Chang, S. J., Lei, Z., Allen, G., and Bommathanahalli, A. 2008. Grid-enabled sawing optimization: from scanning images to cutting solution. In Proceedings of the 15th ACM Mardi Gras Conference: From Lightweight Mash-Ups To Lambda Grids: Understanding the Spectrum of Distributed Computing Requirements, Applications, Tools, infrastructures, interoperability, and the incremental Adoption of Key Capabilities (Baton Rouge, Louisiana, January 29 - February 03, 2008). MG '08. ACM, New York, NY, 1-8. DOI= http://doi.acm.org/10.1145/1341811.1341829
3. Promita Chakraborty, Gabrielle Allen, Zhou Lei, John Lewis, Adam Lewis, Ian Chang-Yen, Itthichok Jangjaimon, Nian-Feng Tzeng, An Integrated Grid Portal for Managing Energy Resources, Proceedings of the Third IEEE International Conference on e-Science and Grid Computing, Bangalore, India, December 10th to 13th, 2007.
4. Xin Li, Zhou Li, Christopher White, Gabrielle Allen, Guan Qin, Frank T-C. Tsai, Grid-Enabled Ensemble Subsurface Modeling, Proceedings of The 19th IASTED International Conference on Parallel and Distributed Computing and Systems (PDCS 2007), November 19–21, 2007, Cambridge, Massachusetts, USA.
5. Zhifeng Yun, Samuel J. Keasler, Maoyuan Xie, Zhou Lei, Bin Chen and Gabrielle Allen. {\em An Innovative Simulation Approach for Water Mediated Attraction Based on Grid Computing}. Proceedings of International Multi-Symposiums on Computer and Computational Sciences 2007 (IMSCCS|07), Iowa City, Iowa, USA, August 13-15.
6. Maoyuan Xie, Fuguo Zhou, Zhifeng Yun, Gabrielle Allen, Tevfik Kosar, and Zhou Lei. Collaborating Mechanical Design Phases Across A Grid. Proceedings of International Multi-Symposiums on Computer and Computational Sciences 2007 (IMSCCS|07), Iowa City, Iowa, USA, August 13-15.
7. Ashwin Bommathanahalli, Maoyuan Xie, Zhifeng Yun, Sun Joseph Chang, Zhou Lei, Gabrielle Allen, TOPSAW Sawing Optimization Analysis Using Grid Computing, Proceedings of International Multi-Symposiums on Computer and Computational Sciences 2007 (IMSCCS|07), Iowa City, Iowa, USA, August 13-15, (2007). [Download]
8. "Louisiana: A Model for Advancing Regional e-Science through Cyberinfrastructure," Daniel S. Katz (LSU), Gabrielle Allen (LSU), Ricardo Cortez (Tulane), Carolina Cruz-Neira (ULL), Les Guice (LaTech), Shantenu Jha (LSU), Ramesh Kolluru (ULL), Tevfik Kosar (LSU), Lonnie Leger (LSU), Charlie McMahon (LSU), Jarek Nabrzyski (LSU), Ed Seidel (LSU), Greg Speyrer (LC&TCS), Michael Stubblefield (SUBR), Brian Voss (LSU), Scott Whittenburg (UNO), submitted to the 2008 UK e-Science All Hands Meeting.
9. "Workflow Task Clustering for Best Effort Systems with Pegasus," G. Singh, M.-H. Su, K. Vahi, E. Deelman, B. Berriman, J. Good, D. S. Katz, and G. Mehta, Proceedings of 15th Mardi Gras Conference, 2008.
10. Christian D. Ott, Erik Schnetter, Gabrielle Allen, Edward Seidel, Jian Tao, and Burkhard Zink. A case study for petascale applications in astrophysics: Simulating Gamma-Ray Bursts. In Proceedings of the 15th ACM Mardi Gras conference: From lightweight mash-ups to lambda grids: Understanding the spectrum of distributed computing requirements, applications, tools, infrastructures, interoperability, and the incremental adoption of key capabilities, number 18 in ACM International Conference Proceeding Series, Baton Rouge, Louisiana, 2008. ACM. (PDF, 9 pages, 886.2 kbyte) (doi:10.1145/1341811.1341831)

11. Erik Schnetter, Christian D. Ott, Peter Diener, and Christian Reisswig. Astrophysical applications of numerical relativity — from Teragrid to Petascale. The 3rd annual TeraGrid Conference, TeraGrid '08 (accepted), 2008.
12. Erik Schnetter. Multi-physics coupling of Einstein and hydrodynamics evolution: A case study of the Einstein Toolkit. CBHPC 2008 (Component-Based High Performance Computing) (submitted), 2008.
13. Book chapter: Erik Schnetter, Christian D. Ott, Gabrielle Allen, Peter Diener, Tom Goodale, Thomas Radke, Edward Seidel, and John Shalf. Cactus Framework: Black holes to gamma ray bursts. In David A. Bader, editor, Petascale Computing: Algorithms and Applications, chapter 24. Chapman & Hall/CRC Computational Science Series, 2007.
14. Huang, Wei; Aboul-ela, Fareed; Jha, Shantenu; Boyapati, Vamsi. Computational study of conformational switching of s-box riboswitch. Poster at 235th ACS National Meeting, New Orleans, LA, United States, April 6-10, 2008 (2008), BIOL-182. [PDF] [HTML as following] http://www.cct.lsu.edu/~whuang/index_files/p1148885.pdf
15. "Clouds Provide Grids With Higher Levels of Abstractions and Support for Explicit Usage Modes", submitted to, Concurrency and Computing: Practise and Experience (2008) {\href{http://www.ogf.org/OGF_Special_Issue/cloud-grid-saga.pdf}{URL}}
16. "Large Scale Computational Science on Federated Grids: The Role of Switched Optical Networks", In print, to appear in Future Generation Computing Systems
17. "Distributed I/O with PARAMEDIC", Proceedings of the International Supercomputing Conference 2008
18. Developing Adaptive Scientific Applications with Hard to Predict Runtime Resource Requirements, Proceedings of TeraGrid 2008
19. Application Level Interoperabiloity Using SAGA, pp 584-59, International Workshop on Interoperation and Interoperabiltiy in Grids, Held in conjunction with e-Science 2007, Bangalore (India) ISBN: 978-0-7695-3064-2, DOI: 10.1109/E-SCIENCE.2007.39
20. Design and Implementation of Network Performance Aware Applications Using SAGA and Cactus, pp 143-150, IEEE Conference on e-Science 2007, Bangalore, ISBN 978-0-7695-3064-2, DOI: 10.1109/E-SCIENCE.2007.28
21. ``Rapid, Accurate, and Precise Calculation of Relative Binding. Affinities for the SH2 Domain Using a Computational Grid'' J. Chem. Theory Comput.; 2007; 3(3) pp 1193 - 1202; (Article) DOI: 0.1021/ct6003017

Technical reports:

1. Gabrielle Allen, Elena Caraba, Tom Goodale, Yaakoub El Khamra, and Erik Schnetter. A scientific application benchmark using the Cactus Framework. Technical report, Center for Computation & Technology, April 2007. (PDF, 6 pages, 539.9 kbyte)
2. John Shalf, Erik Schnetter, Gabrielle Allen, and Edward Seidel. Cactus as benchmarking platform. Technical Report CCT-TR-2006-3, Louisiana State University, 2007.
3. Erik Schnetter, Gabrielle Allen, Tom Goodale, and Mayank Tyagi. Alpaca: Cactus tools for application level performance and correctness analysis. Technical Report CCT-TR-2008-2, Louisiana State University, 2008.

From LA Tech:

1. N. Simicevic, International Workshop on EMF Dosimetry and Biophysical Aspects Relevant to Setting Exposure Guidelines, 20 - 22 March 2006, Berlin, Germany.

2. N. Simicevic, 2008 Asia-Pacific Symposium on Electromagnetic Compatibility in conjunction with the 19th Intern. Zurich Symposium on Electromagnetic Compatibility, May 19 - 22, 2008 Singapore.

3. Veeramallu R., Kunjamon A. and Mainardi D.S., "CO_2 Conversion to Methanol and Ammonia Activation of Methanol Dehydrogenase Enzyme upon Methanol Binding", Proceeding paper of the National conference of the American Institute of Chemical Engineers (AIChE), Salt Lake City, UT, Nov 4-9, **2007**.

4. Idupulapati N.B. and Mainardi D.S., "Methanol Electro-Oxidation By Ion-Modified Methanol Dehydrogenase Enzymes", Proceeding paper of the National conference of the American Institute of Chemical Engineers (AIChE), Salt Lake City, UT, Nov 4-9, **2007**.

5. Keeton K.L and Mainardi D. S. "Characterization Of Mediators Proposed To Better Facilitate Electron Transfer In Methanol Dehydrogenase Enzymatic Fuel Cells", Proceeding paper of the National conference of the American Institute of Chemical Engineers (AIChE), Salt Lake City, UT, Nov 4-9, **2007**.

6. Keeton K.L and Mainardi D. S. "Nano/bio-Systems Modeling In Undergraduate and Graduate Education Using Gaussian '03 and Material Studio", Proceeding paper of the National conference of the American Institute of Chemical Engineers (AIChE), Salt Lake City, UT, Nov 4-9, **2007**.

7. Dathara P.G.K and Mainardi D. S. "Modeling Effects of Titanium Dopants on Hydrogen Adsorption/Desorption Kinetics by Sodium Alanates", Proceeding paper of the National conference of the American Institute of Chemical Engineers (AIChE), Salt Lake City, UT, Nov 4-9, **2007**.

8. Ghouri M. M. and Mainardi D. S. "Carbon Based Lithium Metal Hydrides for Hydrogen Storage", Proceeding paper of the National conference of the American Institute of Chemical Engineers (AIChE), Salt Lake City, UT, Nov 4-9, **2007**.

From SUBR, two drafts interfacing material and computer science were written in order to be submitted.

Drs. Kolluru, Smith, and Stewart (UL Lafayette) and Dr. Geoff Parker (Tulane University) are developing a paper in the area of supply chain and critical infrastructure interdependencies. This paper represents an intersection of computer science, business and engineering as domains.

b) Inter-university Papers, Projects and Proposals

Proposals collaborating between LONI universities:

1. LA EPSCoR Pfund program by NSF/LA-BOR, “Plasmonics substrates fabricated nonlithographically for fluorescence and Raman signal enhancement,” July 01, 2008 – June 30, 2009. --> LA Tech and LSU are involved and collaborate for the proposal. LSU: Tae-Woo Lee (IT consultant at CCT), LA Tech: Long Que (Prof. at LA Tech). Status: approved.
2. NSF ECCS-EPDT program, "Collaborative research: MEMS-based optical antenna near-field pobes for nanoscale imaging and spectroscopy," Sep. 01, 2008 - Aug. 31. 2011. --> LA Tech and LSU are involved and collaborate for this proposal. LSU: Tae-Woo Lee (IT consultant at CCT). LA Tech: Long Que (Prof. at LA Tech). Status: pending.
3. "HPCOPS: The LONI Grid – Leveraging HPC Resources of the Louisiana Optical Network Initiative for Science and Engineering Research and Education," $2M funded by NSF over two years, LONI, LSU, LaTech, SUBR, Tulane, ULL
4. "Leadership Class Scientific and Engineering Computing: Breaking Through The Limits," $200M funded by NSF over 4 years, U. of Illinois, LSU, IBM, RENCI, GLCPC, U. Michigan, LANL, UIC, Iowa State, Shodor, ANL
5. "The LONI Institute: Advancing Biology, Materials, and Computational Sciences for Research, Education and Economic Development," $7M funded by LA BOR over 5 years, LSU, LaTech, SUBR, Tulane, ULL, UNO
6. "MRI: CRON: Development of a Cyberinfrastructure Reconfigurable Optical Network for Large-Scale Scientific Discovery," $496K funded by NSF over 3 years, LSU, SUBR,

Proposals collaborating within LSU (no inter-university) but using LONI systems.

1. DARPA QuEST program, "Theory, design, and modeling of entangled photonic devices for quantum informatics and technologies," July 01, 2009 - Jun. 30, 2013. --> collaboration between CCT and Physics Department in LSU. Status: pending.

Proposals collaborating among LSU and non-LONI universities, but using LONI systems.

1. NIH-NIBIB R01, "Single nanoparticle-surface plasmon resonance imager for label-free imaging of biological structures at nanoscale resolution," Jan. 01, 2009 - Dec. 31, 2012. --> collaboration between CCT at LSU, Univ. of Delaware, and Purdue. Status: pending.

Proposals Submitted but not funded:

1. "CI-TEAM Demonstration Project: Southern US Collaboration for Cyberinfrastructure Enhancement and Educational Development (SUCCEED) Regional Training Program," submitted for $250K over 2 years to NSF, collaborators: Texas Tech, SURA, LaTech, LSU, UTEP, U. Ark., U. Oklahoma, UAB,
2. "Delta: A Petascale Environment for Scientific Discovery," submitted for $30M over 4 years to NSF, collaborators: LSU, LONI, SURA, U. Illinois, University College

London, U. Texas, Brown, U. Penn., Florida Atlantic, Ohio State, Princeton, ORNL, SUBR,

Submitted Presentations:

1. "Louisiana: A Model for Advancing Regional e-Science through Cyberinfrastructure," Daniel S. Katz (LSU), Gabrielle Allen (LSU), Ricardo Cortez (Tulane), Carolina Cruz-Neira (ULL), Les Guice (LaTech), Shantenu Jha (LSU), Ramesh Kolluru (ULL), Tevfik Kosar (LSU), Lonnie Leger (LSU), Charlie McMahon (LSU), Jarek Nabrzyski (LSU), Ed Seidel (LSU), Greg Speyrer (LC&TCS), Michael Stubblefield (SUBR), Brian Voss (LSU), Scott Whittenburg (UNO), submitted to the 2008 UK e-Science All Hands Meeting.
2. "Introduction to the TeraGrid," Daniel S. Katz (LSU/LONI), Phil Andrews (UT-NICS), Jay Boisseau (TACC), John Cobb (ORNL), Kelly Gaither (TACC), David Hart (SDSC), Matt Heinzel (U. Chicago), Scott Lathrop (U. Chicago/ANL), Michael Levine (PSC), Lee Liming (U. Chicago/ANL), Rich Loft (NCAR), J. P. Navarro (U. Chicago/ANL), Tony Rimovsky (NCSA), Sergiu Sanielevici (PSC), Mark Sheddon (SDSC), Carol Song (Purdue), Rick Stevens (U. Chicago/ANL), Craig Stewart (Indiana), John Towns (NCSA), Nancy Wilkins-Diehr (SDSC), submitted to the 2008 UK e-Science All Hands Meeting.

Accepted Papers:

1. "Distributed I/O with ParaMEDIC: Experiences with a Worldwide Supercomputer," P. Balaji, W. Feng, H. Lin, J. Archuleta, S. Matsuoka, A. Warren, J. Setubal, E. Lusk, R. Thakur, I. Foster, D. S. Katz, S. Jha, K. Shinpaugh, S. Coghlan, D. Reed, Proceedings of 23rd Annual International Supercomputing Conference (ISC'08), 2008.
2. "Workflow Task Clustering for Best Effort Systems with Pegasus," G. Singh, M.-H. Su, K. Vahi, E. Deelman, B. Berriman, J. Good, D. S. Katz, and G. Mehta, Proceedings of 15th Mardi Gras Conference, 2008.

LA Tech papers involving collaboration with other universities:

1. L. Pasumansky, C. J. Collins, L. M. Pratt, N.V. Nguỹên, B. Ramachandran, and B. Singaram, "Solvent and temperature effects on the reduction and amination reactions of electrophiles by lithium dialkylaminoborohydrides," J. Org. Chem. 72, 971-976 (2007). (collaborating institutions: UC, Santa Cruz; Fisk University, University of Pedagogy, Ho Chi Minh City, Vietnam, and Louisiana Tech)

2. 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," J. Org. Chem. (submitted). (collaborating institutions: LA Tech, University of Pedagogy, Ho Chi Minh City, Vietnam, and Fisk University)

3. C. D. Wick and L. X. Dang, "Molecular Dynamics Study of Ion Transfer And Distribution at the Interface of Water and 1,2-Dichloroethane," Journal of Physical

Chemistry C 112 (2008) 647-649. Cover article. (collaborating institutions: LA Tech, University of Pedagogy, Ho Chi Minh City, Vietnam, and Fisk University)

4. C. D. Wick and L. X. Dang, "Recent Advances in Understanding the Transfer of Polarizable Ions Across Aqueous Interfaces," Chemical Physics Letters 458 (2008) 1. Invited Review, Cover article. (collaborating institutions: LA Tech, University of Pedagogy, Ho Chi Minh City, Vietnam, and Fisk University)

Dr. Ramachandran's project on organolithium compounds is a collaboration between LA Tech and Fisk University, while his project on acidities of aromatic hydrocarbons is a collaboration between LA Tech, ULM, and GSU.

UL Lafayette researchers Drs. Kolluru, Smith, Chu, Raghavan, Cruz-Neira, and Gottumukkala collaborated with researchers from LSU (CCT and Stevenson Disaster Management Institute) to submit a proposal to the DHS for the establishment of a Center of Excellence for Command, Control and Interoperability.

1.IV.c) Visits to National Labs

From LSU the following personnel visited a National Laboratory.

- Elena Caraba (Undergraduate), LBL in Summer 07, ANL in Summer 08
- Gayathri Namala (Grad), ANL Summer 08
- Mehmet Balman (Grad), Los Alamos National Laboratory, Summer 08
- SIs Erik Schnetter, and Werner Benger and visited LBL last autumn. They discussed remote visualization and visual debugging with John Shalf (LBL) and Hank Childs (LLNL). Another topic was automatic code optimization for stencil-based codes (John Shalf). Both were in the context of the Alpaca project at LSU.

At LA Tech, the High Energy Physics group (Dick Greenwood, Lee Sawyer, Markus Wobisch) are part of the D0 collaboration at FermiLab and also the ATLAS experiment at CERN, Geneva. Their student, Ram Dhullipudi, has visited FermiLab this year, and is leaving for CERN in a few days. The HEP group is also one of the heaviest users of LONI resources.

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.	4 courses used LONI (Sec. 1.V.a).
Statewide training	Number of training workshops, people	Initially 2 HPC & CSs workshops offered per	30 tutorials (204 attendees) and 5

	trained	year, increasing to 4 by Y5; at least 50 people trained each year, 400 total	workshops (166 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	N/A

The LI staff computational scientists will work 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 will be based on overlaps between various partnerships, such as application-based workshops and toolbased workshops.

1.V.a) HD Video Courses

As part for a transformative education program, some institutions have offered HD video courses.

At LSU, Dr. Thomas Sterling taught the course "High-Performance Computing: Models, Methods and Means" in Spring of 2007, and it was the first of its kind in the United States. Sterling taught the course at LSU, and broadcast it across the 10-Gigabit-per-second Louisiana Optical Network Initiative (LONI) to sites in Louisiana, Arkansas, North Carolina and the Czech Republic. Sterling taught his course again in the Spring 2008 semester, with four additional universities – Louisiana Tech University, University of Arkansas-Fayetteville and Little Rock campuses and Masaryk University in the Czech Republic -- signed on to participate. Students from LA Tech Students who took the course received graduate credit for CSC 557: Selected Topics in Computer Science.

In Spring 2008, LSU offered a course in Spring 2008 that used the same setup in reverse. Students were able to take the University of Illinois – Chicago's video game design class, offered at LSU as both a computer science course (CS 4700) and an arts course (ART 4020.)

Dr. Gabrielle Allen at LSU offered the video game design course for the first time during the fall 2007 semester, and Allen said it was so successful, the University offered it again in the spring.

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

Here, we provide a list of the workshops and tutorials LSU organized, as well as the number of participants. Even though we only list the events after Fall 2007, these workshops and tutorials have been offered previously as well. Many faculty, research associates, graduate students from across the State attended and have received training on LONI.

Semester	Training	No. Enrolled
	Tutorials	
Fall 2007		
4-Sep	Introduction to Linux	9
10-Sep	Intermediate Linux	12
12-Sep	Introduction to HPC & LONI Linux Clusters	8
18-Sep	Introduction to HPC & LONI P5s	5
26-Sep	Introduction to MPI	14
2-Oct	Introduction to OpenMP	6
3-Oct	Introduction to Linux	6
8-Oct	Configuring your HPC & LONI Linux Clusters Linux Account	4
15-Oct	Introduction to LaTeX	5
17-Oct	Configuring your LSU & LONI P5 Account	3
23-Oct	Introduction to Vi	7
24-Oct	Introduction to MPI	11
24-Oct	Introduction to HPC & LONI Linux Clusters	5
30-Oct	Introduction to OpenMP	7
6-Nov	Intermediate MPI	9
28-Nov	MPI part 3	2

Fall 2007	Total	113
	Workshops	
October 11 & 12	LONI HPC Workshop	35
	(2 days at Louisiana Tech)	
Nov. 27 & 28	LONI HPC Workshop	28
	(2 Days at ULL)	
Summary		63
	113 people were trained in Fall 2007 in 16 tutorials and 64 people attended 2 workshops.	

Semester	Training	No. Enrolled
	Tutorials	
Spring 2008		
28-Jan	Introduction to Linux	6
30-Jan	Introduction to Vi	5
6-Feb	Introduction to HPC & LONI P5s	7
13-Feb	Introduction to HPC & LONI Linux Clusters	7
11-Feb	Intermediate Linux	5
20-Feb	Introduction to MPI	5
27-Feb	Introduction to OpenMP	6
12-Mar	Intermediate OpenMP	6
26-Mar	Introduction to Linux Clusters Compilers & Optimization	4
2-Apr	Intermediate MPI	7
16-Aprl	Tuning MPI Performance on Pelican	8

9-Apr	IBM P5 Compilers and Optimizations	3
22-Apr	Introduction to Hybrid MPI/OpenMP	7
2-Apr	Haskell Programming	15
Spring 2008	Total	91
	Workshops	
11 & 12-March	LONI HPC Workshop	44
	(2 days at LSU: 14 tutorials)	
23 & 24-April	LONI HPC Workshop	22
	(2 days at UNO: 14 tutorials)	
25 & 26-Mar	LBRN Computational Biology Workshop	36
	(2 days at LSU)	
Summary		
	91 people were trained in Spring 2008 in 14 tutorials, and 102 people attended 3 workshops	

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

During Summer 2007, the LSU Center for Computation & Technology hosted a high-performance computing "boot camp" for 25 students from five area high schools. The bootcamp was called “Beowulf Bootcamp”, and from July 30 to Aug. 3 students got a crash course in the basics of supercomputing. The camp is designed around the work of Thomas Sterling, co-inventor of the Beowulf class "cluster" comprising today's supercomputers

In LA Tech, the week-long “CyberCamp” for High School students concluded on June 13. For more details, please contact Galen Turner at gturner@latech.edu

2. CONTRIBUTIONS

The LI is still in the formative stages as we hire personnel. We do not expect its faculty to be fully in place (and therefore its contributions to the state research and education capacity will not be fully felt) until Y3 and beyond. However, at this stage the LI already has made important contributions:

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

Through a collaborative search procedure we have already hired five faculty who will begin arriving in Y2 (with 7 more to be hired in Y2-3). These faculty are outstanding, and have been attracted to the state through activities on LONI and through LI member cooperation. All are highly computationally oriented, and some are international leaders in their fields. For example, Prof. Jarrell is an APS Fellow and leader of several international collaborations. During the recruitment phase, members of the LI sites discussed candidates, coordinated recruitment across the universities, and even participated in interviews. The result is that these new faculty are already in discussions with various LI members about collaborative, multi-institutional research projects that utilize LONI, setting the stage for larger collaborative funding projects in the future. These faculty will then be effective in recruiting the second round of faculty in Y2.

Through recruitment of the four computational scientists (with two more still to be recruited), the existing faculty have come to know each other and the interests of each site. These scientists are only just arriving and have not yet become involved in the advanced projects across the state, but will be by fall, 2008. This contributes directly to the research and educational capacity of the state, by making the projects our faculty carry out more advanced, and grant proposals we write more competitive. These staff will also help train the university base on cyberinfrastructure (CI) we develop, making them more competitive as well. Finally, these staff will be critical to advances in corporate partnerships as they are developed, as they will be able to support research projects by companies that are carried out, using LONI and other CI we develop and deploy, in collaboration with our LI university partners.

Finally, in supporting our graduate students for work on LONI, we are clearly supporting the state research and education capacity.

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

As reported above, the pre-existing LI faculty and staff (the PIs and SIs) have received external funding for numerous projects during the first year. Most of this funding was already applied for by the faculty in advance of the start of the LI project, but we expect the collaborations developed will be strengthen and enhanced as the LI gains new members in Y2 and beyond. The most important of these projects from the point of view of

infrastructure for the state is the $12M CyberTools project, which we expect will provide advanced CI for the entire state, not only the LI members. The $2.2M NSF HPCOPS project brings the LONI infrastructure to the TeraGrid, which is the NSF's national backbone for advanced CI. This award funds 7 staff positions to better develop and support the LONI environment, while integrating this national environment with the state. This makes it much easier for all state researchers to take advantage of the national CI. Together, these two awards lay a strong foundation for future projects.

2.III. Infrastructure.

Both the HPCOPS and CyberTools awards are providing advanced CI for the state to build on.

2.IV. Economic Development.

As described above, companies have been formed by the PIs and corporate partnerships are being explored, even at this very preliminary stage of the development of the LI. For example, deep discussions have been held with Schlumberger for a series of pilot projects with staff and faculty at LSU, which if funded would make use of the projects funded by CyberTools and CCT. This in an example of the kinds of economic development partnerships that we expect to develop in the future once the LI is up and running.

3. PROJECT REVISIONS.

We do not at this time expect any revisions to the project deliverables. As additional faculty and staff are recruited, we expect to continue on track to deliver what was originally promised. However, the PI (Seidel) has accepted the position of Director of the Office of Cyberinfrastructure at NSF, and his time for advancing the LI will be very limited. This will impact the LI, and we are in discussion on how to handle this as we move forward.