


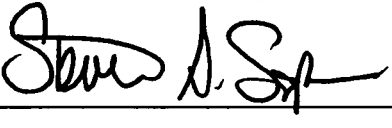
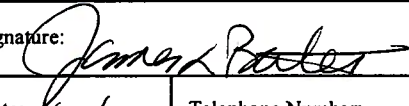
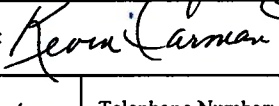
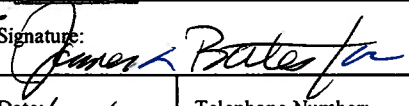


**COVER PAGE FOR POST-KATRINA SUPPORT FUND INITIATIVE
PRIMARYLY RESEARCH SUBPROGRAM PROPOSALS
BOARD OF REGENTS SUPPORT FUND, FY 2006-07**

005PKSFI-R-07

1. Submission Discipline: G Biological Sciences <input checked="" type="checkbox"/> Information Technology G Materials Science (check only one)				(For BoR Use Only) Application Number:	
2. Name(s) of Lead Submitting Institution of Higher Education: Louisiana State University (Include Branch/Campus/Other Components)					
3. Address of Lead Institution of Higher Education: (Include Dept/Unit, Street Address/P.O. Box Number, City, State, Zip Code) Louisiana State University, 320 Thomas Boyd, Baton Rouge, LA 70803					
4. Title of Proposed Project: The LONI Institute: Advancing Biology, Materials, and Computational Sciences for Research, Education, and Economic Development					
5. Proposed Duration: (Circle # of Yrs.) 1 2 3 4 5		6. Funds Requested \$ \$14,730,021		P-KSFI Year 1: \$	ESIP: \$
				Project Total: \$14,730,021	
7. Name(s) of Partnering Institution(s) Louisiana State University, Louisiana Tech University, Southern University, Tulane University, University of Louisiana at Lafayette, University of New Orleans					
8. Does This Proposal Contain Confidential or Proprietary Information Which Falls Into a Category Described in R.S. 44:4(16)? YES <input type="checkbox"/> X NO <input checked="" type="checkbox"/> (NOTE: If YES, the proposal MUST be appropriately marked.)					
By signing and submitting this proposal, the signators are certifying that: (1) the proposed project has not already been funded/is not currently being funded/has not been promised funding; (2) this proposal has been reviewed and approved by an Institutional Screening Committee; and (3) the institution and the proposed project are in compliance with all applicable Federal and State laws and regulations, including, but not limited to, the required certifications set forth in: (a) Grants for Research and Education in Science and Engineering, NSF Grant Proposals Guide (GPG), NSF 03-2, effective 10/1/02, and (b) 45CFR 620, Subpart F (Requirements for a Drug-Free Workplace).					
Name/Title/Institution		Dept./E-mail address/Telephone Number		Signature	
LSU P/PI Edward Seidel Director, Center for Computation & Technology Floating Point Systems Professor		Center for Computation & Technology and Department of Computer Science and Department of Physics and Astronomy Louisiana State University, Baton Rouge, LA (225) 578-7877 eseidel@lsu.edu			
LSU Co-PI Harold Silverman Professor Executive Vice Chancellor, Academic Affairs Dean, Graduate School, Interim Provost		Louisiana State University Department of Biological Sciences/ Academic Affairs 135 Thomas Boyd 225-578-1519 cxsilv@lsu.edu			
LSU Co-PI Tevfik Kosar Assistant Professor		Louisiana State University Department of Computer Science and Center for Computation & Technology (225) 578-9483 kosar@lsu.edu			
LSU Co-PI Steven A. Soper Professor, Chemistry Director, Center for BioModular Multi-Scale Systems		Louisiana State University Department of Chemistry CBM2 229 Choppin (225) 578-1527			
Other Co-PIs SEE ATTACHED PAGES FOR EACH ADDITIONAL INSTITUTION		SEE ATTACHED PAGES FOR EACH ADDITIONAL INSTITUTION		SEE ATTACHED PAGES FOR EACH ADDITIONAL INSTITUTION	
Campus Head or Authorized Institutional Representative		Dean*		Authorized Fiscal Agent	
Name/Title: (type or print) James L. Bates Dir. Office of Sponsored Programs		Name/Title: (type or print) Kevin Carman, Dean, College of Basic Sciences		Name/Title: (type or print) Jerry Baudin, VC Finance & Admn. Services	
Signature: 		Signature: 		Signature: 	
Date: 3/15/07	Telephone Number: (225) 578-3386	Date: 3/14/07	Telephone Number: 578-4201	Date: 3/15/07	Telephone Number: (225) 578-3386

multiple deans from the lead institution are involved in project activities, the dean with authority over the primary submitting department will serve as signatory for all

PROJECT SUMMARY

Name of Lead Institution (Include Branch/Campus): Louisiana State University
Name(s) of Partnering Institution(s) (Include Branch/Campus): Louisiana State University, Louisiana Tech University, Southern University, Tulane University, University of Louisiana at Lafayette, University of New Orleans
Principal Investigators: Edward Seidel , Tevfik Kosar, Harold Silverman, Steven Soper (LSU) Leslie Guice , Box Leangsuksun , Bala Ramachandran, Neven Simisevic (Louisiana Tech University) Habib Mohamadian , Dwayne Jerro, Perpetua Muganda, Michael Stubblefield (Southern University) Laura Levy , Ricardo Cortez, Donald Gaver, John Perdew (Tulane University) Ramesh Kolluru , Magdy Bayoumi, Devesh Misra, Joe Neigel (University of Louisiana – Lafayette) Scott Whittenburg , Vassil Roussev, Stephen Winters-Hilt (University of New Orleans)
Title of Project: The LONI Institute: Advancing Biology, Materials, and Computational Sciences for Research, Education, and Economic Development
<p>Abstract (DO NOT EXCEED 250 WORDS):</p> <p>Computational science (CS) is revolutionizing research, education, and economic development. Both biology and materials science depend on profound advances in computation. We propose the creation of the <i>LONI Institute (LI)</i>, a world-class consortium of dozens of collaborating faculty and researchers spanning six universities that will powerfully enhance the state's scientific capacity. Building on strengths of our existing multidisciplinary and multi-institutional group, <i>LI</i> will include twelve new computational biology and materials faculty, six new CS faculty to develop common computational tools and algorithms, and an additional six new faculty from partner commitments. <i>LI</i> builds the intellectual capital critically needed to drive the \$25M/year Vision 2020 investment and the \$50M LONI infrastructure project.</p> <p>Together, LSU, LaTech, UL–Lafayette, SUBR, UNO, and Tulane will:</p> <ul style="list-style-type: none">• Create 24 new faculty positions in CS, 18 funded 50% by P-KSFI• Integrate 28 existing faculty with summer salary (<i>annually</i>)• Create 36 graduate fellowships• Recruit six <i>LI</i> staff computational scientists for training and development of 7 dozen CS and economic development projects• Fund scientific and economic development coordinators <p>We request \$14M over five years, matched by over \$16M from <i>LI</i> members; <i>LI</i> will be self-sustaining afterwards.</p> <p>With a dynamic and talented workforce, LED, Council on Competitiveness, and national partners, <i>LI</i> will drive Louisiana economic development. Similar efforts in Illinois produced an estimated trillion-dollar impact on the world economy, generating more than \$120M in corporate partnerships, \$400M in grants, and spawning numerous companies. <i>LI</i> leadership</p>

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1 Goals and Objectives

We propose a statewide “*LONI Institute*” (*LI*), with the goal of being a self-sustaining, growing economic development powerhouse focused on computational and scientific research essential for solving challenging problems in materials science and biology. The *LI* will be built on foundations laid by the \$25M annual State Vision 2020 IT initiative and the \$50M Louisiana Optical Network Initiative (LONI), which already connects *LI* members with 40-Gbit optical links (Sec. A.2,C). Reaching far beyond the scope of a single research problem, *LI* will provide major scientific and economic benefits in areas important to Louisiana.

1. Talented Workforce. *LI will recruit dozens of excellent faculty, staff, and students, and train hundreds of others, catalyzing the development of a highly skilled IT-oriented workforce crucial for economic development.* In year one (Y1), 28 existing faculty from campuses across the State, 10 new faculty, 6 new computational scientists, and 12 new graduate students will be active in significant projects at the interface of computational sciences (CSs), materials, biology, and other fields, utilizing LONI and national facilities. In all, at least 24 new faculty will be recruited, and hundreds of other faculty and students will be trained in the use of LONI and involved in advanced projects. Additional faculty, in other disciplines, will join the *LI* as funding becomes available. The university-based workforce in CSs will be significantly enlarged. Partnerships with national labs and other leading corporate and academic centers will be greatly enhanced (see Berman, Booher, Boisseau, Dunning, Jursik, Simon, Smarr, Stevens letters).

2. Competitiveness. *State research institutions will become significantly more competitive for federal funding, recruitment and retention of the best people, and attracting companies.* By Y2, 24 CS, biology and materials projects will be competitive for national computing resources (a ten-fold increase from two years ago). Each year, another 24 projects will be similarly competitive, and by Y5, dozens of graduate students will be supported by federally funded projects in CSs. Large projects will be commonplace, bringing potentially in excess of \$100M in new federal funds for CS projects, and national facilities, STCs, and ERCs.

3. Educational System. *Education will be transformed with CSs infused into the curriculum at all levels, in many disciplines.* In the first year, four statewide classes in CSs and applications will be taught collaboratively by the best *LI* faculty; dozens of high school and university students, staff, and faculty will be trained in the use of LONI facilities. By midway, *LI* will have submitted numerous IGERT proposals in CSs and application areas, leading to new curricula. By the end of the project, hundreds of students and faculty will be trained in interdisciplinary CSs, dozens of classes will be taught annually over HD video, and CS will play a fundamental role in the broader curriculum.

4. Economic Development. *These activities will be harnessed for economic development for Louisiana, with university-industry cooperative research programs and centers of excellence flourishing in five years.* One quarter of the in-depth CS projects will be reserved for corporate partnerships, leading to at least six university-industry research projects in Y1. We expect to have developed at least 20 university-industry joint research projects of significant depth in five years, all with the potential to create university-industry research centers (UIRC). We aim for at least six significant new investments from major companies for UIRCs, over 30 industry grants, and dozens of researchers involved in industry internships.

5. Self-sustaining and Growing *LI*. In five years, the *LI* will be self-sustaining and growing, with new faculty in disciplines that go beyond biology and materials, including engineering, coastal & environmental science, and digital media. All members are committed to continuing investments in faculty recruitment and corporate development programs well beyond the program. *The LI will harness and amplify previous investments through cooperation between its members for greatly enhanced research, education, and economic development.*

2 Project Narrative

A Project Rationale

Louisiana's extraordinary investments in its \$25M annual Vision 2020 IT program, and \$50M LONI project, connecting all research campuses and supercomputers with optical networks, create a strong foundation (Sec. C). But it is the *innovative, collaborative use* of such facilities, by leading researchers in computational sciences (CSs), that will significantly advance the State. Individually, the research campuses have been strengthened. *Together, a statewide "LONI Institute" will integrate and amplify these strengths into a world-class scientific and economic development (ED) powerhouse that is far stronger than its individual parts.*

In its 2005 report to President Bush, entitled "Computational Science: Ensuring America's Competitiveness", the Presidential Information Technology Advisory Committee (PITAC) [1] stated *"Computational science – the use of advanced computing capabilities to understand and solve complex problems – has become critical to scientific leadership, economic competitiveness, and national security... computational science is one of the most important technical fields of the 21st century because it is essential to advances throughout society."* Such reports are creating a fundamental realignment of academic and industrial research activities. The NSF has created a new "Office of Cyberinfrastructure", DOE has created the SCIDAC program ("Scientific Discovery through Advanced Computing"), with similar initiatives in NIH. Recent investments have prepared the State to take advantage of such programs, but ***a strong effort in computational sciences (CSs) — with application drivers in computational biology and materials — is needed to leverage these developments for education, research, and ED. A statewide LONI Institute (LI) can enhance and integrate State strengths to become a national leader in these critical future areas.***

The challenges are numerous, deeply affecting all disciplines. NSF's 2006 Blue Ribbon Panel of Simulation-Based Engineering Science (SBES) [2] states *"researchers and educators [agree]: computational and simulation engineering sciences are fundamental to the security and welfare of the United States... We must overcome difficulties inherent in multiscale modeling, the development of next-generation algorithms, and the design... of dynamic data-driven application systems... We must determine better ways to integrate data-intensive computing, visualization, and simulation. Importantly, we must overhaul our educational system to foster the interdisciplinary study... The payoffs for meeting these challenges are profound."* ***Without a strong effort in CSs, the state will not able to meet such challenges.***

PITAC, SBES, and many other reports all conclude that not only are CSs critical to the nation's future, and recommend large increases in funding, but they stress computational biology and materials as among the strongest, overlapping growth areas to be driven by it. SBES states *"...technology may have its greatest societal impact where innovations in modeling and simulation methodologies intersect in innovations in materials,"* while a recent NRC study [3] concludes that *"the impact of computing on biology will be deep and profound and span virtually all areas of life science research"*. A recent NSF panel on Cyberinfrastructure for Materials [4] states *"A revolution in materials is taking place at the bio/nano interface where biology and materials science truly meet... the realization of biology-inspired materials depends on designing biomacromolecules that interact predictably with materials."* ***The LI aligns the State's research institutions to develop coherent world-class programs that combine and augment existing strengths in materials, biology, and CSs, building directly on the recent investments in LONI that tie them together.***

The following two examples demonstrate the powerful coupling between CSs and the biological and physical sciences. The human genome project, arguably the most significant scientific breakthrough in fifty years, owes its success as much to advances in CSs as it does to experiment. It also illustrates the larger emerging trend: *Large-scale simulation and data sets cannot be analyzed and understood in a reasonable time without computational models, data mining, visualizations,*

and other knowledge discovery tools. Computing will advance biology in the 21st century, just as mathematics advanced physics in the 20th century. In materials, we see similar trends. In 1998 the first computational-science based Nobel Prize was awarded to Kohn and Pople, who devised computational methods that form the basis of a large fraction of materials science, including the trillion dollar semiconductor industry.

PITAC identifies three CSs areas critical to the future of research and industrial activities, especially tools for next generation scientific challenges: *scalable software; new computing and network architectures; sensor- and data-intensive applications.* These research areas are fundamental to the *emerging discipline of CSs*, critical to developing new materials and in understanding biological systems. ***The LI will enable the State to build on existing expertise in CSs with new strength in all three areas of realigned federal programs, needed for world-class programs in computational biology and materials.***

In summary, building on recent progress across the State, including statewide IT investments in Vision 2020 and LONI (Sec. C), we propose the creation of a statewide LONI Institute (*LI*) that can fundamentally transform the State research base with a program that will:

- Focus on high priority scientific problems in biology and materials that require, motivate and drive cutting edge CSs. *LI will study research topics already identified as important growth areas for the State, the nation and the global scientific community (Sec. B.1).*
- Recruit 24 top new faculty in computational biology and materials, and CSs, involve many more existing faculty, and create complete training programs for faculty and students alike in these areas. *LI has catalyzed over \$16M of matched funding which will be used to bring attract high-impact faculty through a coordinated recruitment procedure (Sec. B.3).*
- Bring the State to international prominence in the critical emerging discipline of CSs, addressing all three areas emphasized by PITAC. *LI builds on existing investments in compute resources, networks, and people (Sec. A.3,C).*
- Create strategic alignment of the State with major research funding agencies for decades. *The LI consortium has crafted this project to be inline with funding agency directions. A broad and influential advisory committee, and a committed and diligent management council will ensure the project leverages major federal funding opportunities (Sec. B.3).*
- Support and strengthen many other initiatives in areas as diverse as astrophysics, coastal restoration, petrochemicals, and digital arts, resonating with other State efforts. *LI computational scientists will work with State faculty to advance their research (Sec. B.1,B.3).*
- Have ED impact in areas where the State is heavily investing. *LI will develop corporate partnerships at many levels, with student internships, joint industry-university research projects, and industrial centers of excellence, working both locally with Louisiana Economic Development (LED) and nationally with the Council on Competitiveness and partner sites (Sec. B.3).*

A.1 Description of Research Group

The founding *LI* research group contains three dozen Principal (PI) and Senior (SI) Investigators, representing senior university administration (provosts and vice chancellors), CSs, biology, and materials areas, who span six research campuses in Louisiana: Louisiana State (LSU), Louisiana Tech (LA Tech), University of Louisiana at Lafayette (UL Lafayette), Southern (SUBR), Tulane, the University of New Orleans (UNO), the Louisiana Community & Technical College System (LCTC). *LI* also includes LONI staff, director, and chief scientist, and director of LITE. We expect to broaden the project to include other institutions, including medical campuses.

Research projects from the above group will seed the research, education, and economic development (ED) activities of the *LI*, its greatest impact on the State will be through the recruitment of many new faculty, and the training of existing faculty, with expertise in CSs, computational biology

and materials, and through projects to be proposed as the *LI* grows during the first several years. These projects will be carried out by State faculty, working closely through coordinated programs with dedicated staff scientists, students, LONI staff, and with corporate partners.

LI builds on numerous strong existing connections between the investigators, many of which have been catalyzed in the last few years through LONI, and other infrastructure programs. Collaborative activities (Sec. A.2) include: (i) Guice, Levy, McMahon, Seidel, Silverman, Stubblefield, serve on the LONI management council; (ii) Silverman, Cortez, Gaver, Seidel, Soper, Acharya, Allen, Cruz-Neira, Katz, Kosar, Leangsuksun, McMahon, Jha have submitted a \$12M NSF proposal incorporating Soper's \$9M, multi-institutional NSF CBM² bio/materials center; (iii) Silverman, Seidel, Allen, and Dua are part of the \$17M NIH Louisiana Biomedical Research Network (LBRN); (iv) Kosar, Allen, Seidel, McMahon, Acharya, Bishop, Dua, Gaver, Greenwood, Winters-Hilt, and Kolluru are involved in NSF MRI "PetaShare"; (v) Seidel, Gaver, Guice and others, including partner NCSA, have submitted "Delta", a \$70M NSF petascale facility proposal; (vi) McMahon, Cortez, Seidel, Dua, Katz, Allen, Kosar, Jha, Stubblefield submitted a \$5M HPCOPS proposal to NSF seeking to make LONI part of the TeraGrid.

Current faculty, scientists, and administrators in *LI* are listed in Appendix 5, along with their institutes, departments and research interests. Project members have been chosen because of their expertise, proven ability to work together and to effect change in their units, desire to perform cutting edge computational research, and ability to secure large funding.

The *LI* will be augmented and enabled by new members funded by this grant and the associated institutional match: 24 new faculty, 140 summer faculty, 6 full-time computational scientists, 36 graduate assistants, administrative staff including a full time scientific coordinator. Although these new members will be distributed across the *LI* member sites, the project management mechanisms described in Sec. B.3 will ensure tight coordination. Based on the record of achievement and cooperation of the PIs illustrated above, we anticipate many more projects of similar impact to be proposed and funded as the *LI* develops, profoundly transforming the State in research, education, and university-based ED activity.

A.2 Context for Project

Recent State Vision 2020 IT investments have had an enormous impact on the individual campus capabilities in IT based research, on the computational resources available to them, and on their abilities and incentives to work well together. This proposal leverages these strengths. Due to the collaborations established in the last few years, largely through LONI, a number of large scale research projects have been developed, with numerous large scale, multi-institutional collaborative proposals directly in the critical CSs, biology, and materials areas, some of which were listed in Sec. A.1 above. Here we expand on the research directions represented by these and other projects; these recent research directions will be further expanded to illustrate the types of activities that will be carried out in the *LI* in Sec. B.1.

In the area of *computational research infrastructure*, multi-institutional projects led by the investigators include: (i) LONI itself, a \$50M research infrastructure project, conceived and led by the investigators. Within 2 years of its inception, the State has created arguably the most advanced regional computing facility in the nation, with 40-Gbit optical links connecting all six *LI* members, and two medical centers, with nearly 100 TFlops of distributed computing facilities. The investigators have also proposed: (ii) Two successive NSF **"Track 2" petascale computing facility** proposals (roughly \$70M each) to build a national center on top of LONI. LSU and its LONI partners, along with a national alliance that includes LBNL, ANL, NCSA, and RENCi, along with the Southeastern Universities Research Association (SURA) for outreach. Both of these (the second, **"Delta"**, is under review), propose to build a comprehensive petascale computing facility to enable national, leading edge science and engineering. Related to this effort, PI Seidel

is involved (as Co-PI) with NCSA in a (\$200M hardware) proposal (under review) to an NSF **“Track 1” leadership class petascale facility**, to be deployed in 2011, that aims fundamentally to change the complexity and scale of scientific inquiry. All these proposals are distinguished by innovative approaches to creating usable tools for scientific research, and by strong collaborative outreach among science partners; (iii) Two **funded NSF MRI proposals**, led by the PIs, involve literally all *LI* members, develop advanced infrastructure for visualizing data and interacting with complex computing environments in LONI (**VizTangibles**), and provide new petascale, distributed data archive and retrieval systems for applications across the State (**PetaShare**); (iv) **LITE, the Louisiana Immersive Technology Enterprise**, a \$27M (funded) center that brings together research, government and industry leaders who want to explore and learn the latest in immersive visualization and supercomputing technologies. These are *four examples of leading edge research infrastructure that has been proposed or created by the PIs in the last 3 years*; such efforts will not only multiply through the *LI*, they will be driven to produce the highest international level science by the researchers we will train and recruit.

In the area of *CSs and cyberinfrastructure development*, multi-institutional projects led by the PIs include: (i) A \$12M NSF EPSCOR project, **CyberTools**, that will build on LONI to develop a statewide, distributed computing infrastructure for advanced applications, including computational materials and biology (and CBM² below); (ii) a \$3.5M DOE EPSCOR project, **UCoMS** [5], built on LONI, that will create advanced statewide cyberinfrastructure for task farming, monitoring, and computing, particularly in petroleum; (iii) **SCOOP** [6], an integrated project of universities working to build a distributed computing system to forecast hurricanes; (iv) **EnLIGHTened** [7], with four universities collaborating to develop systems to allow users and applications to reserve and configure optical network paths between compute and other resources. EnLIGHTened is also working with Asian and European projects to create world-wide standards for global applications; (v) **Cactus** [8] is problem-solving environment with over 10 years of development at many universities and laboratories in the US and Europe. It was used originally for numerical relativity, but now also is used for reservoir simulations, chemistry, computational biology and CFD; (vi) **SAGA** [9], the Simple API for Grid Applications, creates a standard interface for application programmers to run the same applications on different grid middleware. It is part of the Open Grid Forum, with development occurring at multiple world-wide universities. These six examples illustrate the type of research our team is capable of that leads to practical tools that will enable LONI applications in computational biology, materials and other disciplines to flourish.

In the area of *computational biology and materials*, multi-institutional projects led by the PIs include: (i) **LBRN**: [10] \$17M NIH project, Louisiana Biomedical Research Network (LBRN) to improve the research capabilities of the State by increasing access to research infrastructure, training and mentoring of faculty, graduate and undergraduate students and the development of research collaborations amongst researchers; (ii) **GridChem**: [11] \$3M NSF project, is a virtual organization distributed across Illinois, Texas, Ohio, Kentucky and Louisiana that provides access to HPC resources for commonly used computational chemistry and biology applications with distributed support and services, intuitive interfaces and measurable quality of service; (iii) **CBM²**: [12] the \$9M NSF-funded Center for Biomolecular Center for Multiscale Systems to enable work at the interface between materials and biological systems. CBM² is a collaboration between researchers at LSU (Center for Advanced Microstructures and Devices Chemistry, Biology, and Engineering), the LSU and Tulane Health Science Centers, and Xavier. These current three projects illustrate current research interests and abilities of the PIs to blend education, research, and interdisciplinary CSs in the proposed areas. More details of related science research efforts are provided in Sec. B.1.

In the area of *CSs education*, multi-institutional projects led by the PIs include: (i) an \$3M NSF **IGERT** program [13] in computational fluid dynamics (CFD), led by SI Acharya, that infuses CSs with CFD in a multidisciplinary educational curriculum with applications in computational biology, materials, and other areas. Graduate students are trained through research projects and new courses,

taught by a team of faculty from multiple colleges and LONI member institutions; (ii) **LSU's High Performance Computing (HPC) class** [14] taught by SI Sterling over HD video to classrooms at LA Tech, Arkansas, and Masaryk University (in Brno, Czech Republic). The technology used for this class builds on the EnLIGHTened project [7], and will form the foundation for a transformative education program of the *LI* (Sec. B.1).

In the areas of *corporate partnership development in CSs for ED*, multi-institutional projects led by the PIs include research and educational partnerships with **Microsoft** (for Cactus development, research in computer architecture), **Cisco** (on optical network projects, including EnLIGHTened), **IBM** (joint software development for petascale computing, education programs, optical networks), **Intel** (development of SAGA, Cactus), **Dow** (computational chemical engineering), **Schlumberger** (remote visualization, reservoir simulations, advanced computational science), **Calient** (optical network applications), **AT&T** (optical network applications), **Hewlett-Packard** (Grid computing), **Sun** (Cactus, Grid Computing), **SGI** (Cactus, visualization). The comprehensive industrial partnership program proposed by *LI*, in cooperation with LED and the Council on Competitiveness, will greatly expand and strengthen such partnerships, involving both local and national companies.

A.3 Existing Scientific Excellence

The guiding principle of this proposal is to enhance and collect excellence in research groups that are anchored at each site, which will then be integrated thematically through common needs in CSs, physically and electronically by the LONI Institute.

At **LSU**, Vision 2020 funding created the CCT [15], which has developed world-class groups in CSs and applications [16]. Areas of special strength include grid computing, HPC, computer architecture, computational mathematics, and others. PI Seidel was the 2006 IEEE Sidney Fernbach award winner [17]; SIs Allen and Sterling are Gordon Bell Prize winners; Sterling is the father of the Beowulf cluster. CCT has led national alliances for major (\$70M+) NSF centers. Its future directions can be found at [18]. PI and LSU Provost Silverman is distinguished biologist who has led the state to roughly \$30M in external funding in the last few years, while PI Soper, leading the \$9M CBM² bio/materials center, spearheads efforts in materials.

LA Tech has invested in major facilities and research in IT, biomedical engineering, and nanosystems engineering/science. Special strengths include secure networks and HPC systems, bioinformatics, computational biology, molecular modeling, computational materials, biophysical modeling, and computational high-energy physics. PI Leangsuksun develops fault tolerant and reliable large-scale systems in the HA-OSCAR project; SI Greenwood led LA's participation in the Open Science Grid; SI Mainardi models novel nano/biomaterials for fuel cells; PIs Ramachandran advances the design of future nanoelectronics devices and Simicevic has received international recognition for modeling bioelectromagnetic phenomena. SI Paun models HIV-1 strand R5 protein effects on infected cells. LA Tech is firmly committed to further investments in faculty at the interfaces of the info-bio-nano-related disciplines.

At **SUBR**, the Advanced Materials Research Laboratory was established to strengthen and develop its materials program, with a mission to investigate important problems in materials theory and modeling with novel computational approaches, and develop powerful new tools for materials theory and modeling accelerating their integration into industrial research.

At **Tulane** the Center for Computational Science (CCS), founded by Cortez (PI, Director), Gaver (PI) and Fauci (SI), was created in 2001 with DOE funding to develop and support collaborative CS projects. PI Gaver recently received a \$1.2M NIH center grant to investigate multi-scale problems in the biological sciences, linking faculty from biomedical, chemical, and mechanical engineering, mathematics, and environmental health sciences. This NIH center develops collaborative interdisciplinary projects, and has developed new team-taught courses that link CSs and biological modeling. PI Perdew is an APS Fellow, one of the 100 most cited physicists worldwide,

and developer of methods widely used in materials science.

At UNO the State IT Initiative has stimulated major developments in the areas of materials, CSs, and computational biology. UNO established the Advanced Materials Research Institute (AMRI) with core support staff, five new faculty, and state-of-the-art facilities; a collaborative PhD program in Materials Science and Engineering is pending final approval. PI Roussev is a PI or Co-PI on several pending proposals (NSF, NIH, DoD, and NSA/DHS) totaling over \$4.5M. PI Stephen Winters-Hilt has expertise in using nanopores for cheminformatics.

UL Lafayette has invested in CSs and its applications. PI Kolluru (IT) has received \$20M from NSF, DOE, DoD, ARL, Department of Commerce, State agencies, and industry partners, and holds 12 technology copyrights. PI Bayoumi directs UL Lafayette's Center for Advanced Computer Studies (CACS). SI Cruz-Neira is LITE Director and Chief Scientist, and a designer of the CAVE(TM) Virtual Reality Environment. PI Neigel is a leader in computer-based analysis of DNA and protein data and DNA-based methods for the detection of waterborne organisms. PI Misra is Director of the Center for Structural and Functional Materials.

A.4 Multi-institutional Focus

All six LONI member universities (LSU, LA Tech, SUBR, Tulane, UL Lafayette, and UNO) are fully involved and committed to the *LI*. Their financial commitments, detailed in the project summary, total more than \$16M over five years, and will continue at a level of at least \$2.5M annually thereafter. In terms of new research and training activities created by *LI*:

- 24 new faculty positions are already committed to be created in CSs: one in each of CS, computational biology, and computational materials at each site, six additional at LSU (2 in CS, 3 in Materials, one in Arts and Sciences).
- Over 100 current faculty and 36 graduate students will be supported will be supported to begin CSs research projects.
- 6 staff scientists will be supported to develop 70-90 advanced research and ED projects based on advanced cyberinfrastructure developing across LONI.

This will be achieved through requested research support of less than \$2.8M/year from the BoR, which is very evenly distributed across all institutions. As described in Secs. (B.1, B.3), interdisciplinary research teams will be developed that span multiple institutions, working together to solve complex problems in materials and biology, using common CSs tools deployed across LONI. Strong coordination between research groups, educational programs, and industrial partner programs will be provided by *LI* to ensure focus and success. LCTC (Louisiana Community and Technical Colleges) will participate in industrial outreach and education programs (Sec. B.1).

B Research Plan

B.1 Proposed Work

We discuss the science goals of the *LI*, illustrated by current PI research projects, followed by the description of the recruitment of faculty, computational scientists, students, and the programs to achieve our goals.

Major scientific advances in the next decades will be based upon the ability to simulate and build theoretical frameworks for biological and material phenomena spanning many scales, and to integrate data from different sources into the simulation loop. For example, the ability to take (static) information from genome sequence data and translate that into a customizable medical treatment requires input from (dynamic) real-time simulations and analysis of target drug binding properties. Such predictive capabilities use advanced analytical tools and techniques, which require funda-

mental advances in computational approaches to multiscale science. Multiscale computation – including the broad field of Systems Biology [19, 20] – is characterized by heterogeneous, loosely-coupled program components, and is ideally suited for a distributed computing environment, precisely of the type exemplified by LONI.

An overarching aim of the *LI* is to position the State to be at the forefront of such scientific research, by providing expertise and leadership. The three-track strategy to achieve this goal is based upon aggressively developing statewide, overlapping programs in multiscale computational biology and materials, strongly integrated with a third program in CSs to provide the tools, techniques, and infrastructure to spearhead multiscale science programs. ***By tightly coupling world-class biologists, materials scientists, computational scientists, and LONI's computational infrastructure, we will drive excellence and innovation that will only occur at the intersection of these areas, as stressed in PITAC and other reports (Sec. A).***

The specific scientific work advanced by *LI* will depend largely on the faculty recruited. However, to illustrate future work and to establish our ability to attract the best faculty, we discuss specific exciting projects that are either ongoing, or planned at the *LI* institutions. All such projects will benefit greatly from the *LI* – which will provide core expertise around which to nucleate future statewide, multiscale activity in biology and materials.

Computational Materials: The economic impact of computational materials [21] is around \$100B per year. There is a wide range of ongoing research effort (ranging from pharmaceutical materials to new materials design *in silico*) that will form the basis for expanding the State's capability into innovative and economically relevant areas of computational materials. Current pharmaceutical materials efforts (Tulane) revolve around an NIH grant for designing a carrier formulation for the transcutaneous delivery of vaccines. This requires investigations of transport phenomena and novel material properties using advanced computational techniques and new algorithms. In general, the importance of computational methods in the pharmaceutical industry will increase. Advances in multiscale models and techniques will contribute to progress in other areas of materials science too, for example in the study of conductive polymers (LA Tech) using an approach that couples molecular dynamics (MD) simulation to obtain parameters, that are then used in transport simulations at the micro/macroscale level. Specific areas of material science that we will expand upon include:

Materials Theory, Modeling, Computation, and Analysis: A robust and practical microscopic theory of materials must cover the entire range from atoms and molecules to surfaces and solids. Unfortunately, conventional methods using many-electron wavefunctions are only useful for very small systems. The density functional theory (DFT) of Kohn and Sham [22] is the most widely-used method of electronic structure calculation in materials. SI Perdew (Tulane) is a leader in understanding and improving approximations in DFT incorporating a ladder of approximations in which each rung is characterized by the set of local ingredients used to construct the exchange-correlation energy density at any point in space. Over the last 30 years, this group has derived the first three rungs from known or derived exact constraints, without empirical fitting. Current research is directed towards the fourth rung (hyper-GGA), which will eliminate the remaining largest energy errors of density functionals. As this research area demonstrates, ***the coupling of fundamental physics with CSs will create new approaches for materials design, and represents a model for how theoreticians and computational scientists can collaborate to strengthen each group.***

At UNO, modeling of materials is aimed at understanding the magnetic properties of materials and devices using micromagnetics. Most of the simulations employ a code developed in-house called JaMM [23], or Java MicroMagnetics, which has been made available in the public-domain. ***Computational materials at UNO already supports a spin-off local company, NanoPrism, which synthesizes nanomaterials.***

Surfaces, Interfaces and Nanostructures (Tulane): Surfaces and interfaces are a key for utilizing materials because when materials shrink in size, surface effects can dominate; many of the intrigu-

ing properties of nanomaterials are due to surface effects. ***Computational studies will help to unravel the structural, electronic, and other physical properties of low-dimensional materials and to develop novel techniques for the rational synthesis of nanostructures*** (e.g., through directed self-assembly and new thin film deposition techniques). Potential applications include such diverse fields as (photo-)catalysis, corrosion protection, sensors, micro- and nano-electronics, 'spin'tronics, as well as bio-compatible and bio-inspired materials.

System-on-Chip Design and Integration (UL Lafayette): The UL Lafayette VLSI-SoC lab develops integration methods for CMOS ICs containing signal processing and analog signal conditioning hardware with heterogeneous families of sensors as a single chip or single package solution. HPC and grid resources enable full process simulations and visualization of these designs using detailed physics models. This will be ***critical for LI industrial partners who can access these prefabrication designs and simulations before actually committing them to foundries.***

Computational Modeling of the Mechanical Behavior of Polymer Nanocomposites (UL Lafayette): Polymer nanocomposites are representative of a new class of multiphase nanostructured materials at a scale intermediate between nano- and micro-scale. Polymer nanocomposites exhibit novel and improved properties that are not displayed by the individual phases or by their conventional composite counterparts, such as improvement in mechanical properties like tensile strength, tensile modulus, lower thermal expansion coefficient and flame retardant capability. MD simulations are used to analyze the molecular mechanisms by which nanosized particles reinforce polymer matrix [24], and to investigate technologically feasible and economically acceptable solutions for manufacturing polymer based composites for new applications. ***Investigating interfacial, bulk and composite performance properties requires advanced modeling and computer simulation techniques at micro, nano and intermediate length scales.***

Micro Electro-Mechanical Systems (MEMS) (LSU): MEMS encompass systems that combine mechanical devices, such as actuators, fluidic components or temperature sensors, with electronic circuits and contain essential microstructured elements. As the system footprint is reduced, MEMS may require nanostructures (NEMS). Medical applications of MEMS (BioMEMS) have been identified as the next enabler for MEMS. Research has continued to advance in BioMEMS-related fields, Potential BioMEMS applications include drug discovery, diagnostics, targeted drug delivery, microarrays, DNA sequencing, artificial organs, micro-surgical instruments and tools for point-of-care operation. Recent market surveys estimate that the total world market for BioMEMS will increase from \$14 billion in 2001 to \$38 billion in 2008. Research in BioMEMS/BioNEMS using polymer science & engineering (S&E) are being integrated into several existing State research groups, such as the Macromolecular Studies Group and CBM². Research initiatives will build upon existing efforts of several campuses including LSU, Tulane and UNO. ***Success in the polymer S&E areas outlined below will depend intimately on a diverse range of computational capabilities.***

Polymer Design and Synthesis: We use synthetic expertise to polymerize new monomers, such as peptides, to build functional materials that can be integrated into BioMEMS and BioNEMS devices. Computational efforts in material design will be critical to guide synthetic preparation of novel materials and to model material behavior on the nanometer-scale. In collaboration with the Materials Focus Area of the CCT, which has ***groups that use computational approaches to complex materials problems a research thrust will be to develop a framework to understand and control nano-structural material properties.***

Polymer Rheology and Mixed-Scale Flow: Numerical modeling of manufacturing processes can provide key insights into the local physical characteristics of the product, and can be used to tailor the manufacturing process to improve desired characteristics (strength, homogeneity, dimensional tolerance etc). The modeling of common manufacturing processes (e.g., molding, embossing etc.) requires advanced simulation capabilities. For example, injection molding involves injection of the material, in liquid or semi-liquid form, into a pre-formed mold and allowing the material to solidify.

The simulation must incorporate fluid flow and energy transport, free-interface solidification, a moving solid-liquid interface, property changes during solidification and conjugate heat transfer. Extrusion and embossing both involve the deformation of solid material. ***In order to simulate such multi-scale and multi-physics scenarios, requires advanced tools, algorithms and hardware.***

Polymer (soft-matter) Imaging: High resolution electron microscopy evaluation of polymers and composites allows for the unprecedented imaging, and speciation in many cases, of complex polymer composite systems. Due to the research expertise associated with data acquisition and processing (Kosar), and image reconstruction (Ullmer), that is present in the State, ***we will be one of only a small number of select groups around the world with the needed capabilities to address this burgeoning and pivotal field of polymer imaging.***

Computational Biology: Similar to efforts in materials, the computational biology focus will leverage existing strengths and couple these to advances in CSs. For example, a multidisciplinary Quantitative Biology Initiative (QBI) that will build upon and synergize existing strengths in computational science, structural and evolutionary biology is planned at LSU.

Metagenomics is an emerging field that examines genomes from the perspective of entire ecosystems and the organisms that comprise these systems and will be a specific focus of the QBI; it is an archetypical example of multiscale and systems biology approach requiring coordinated collaboration between CSs and computational biologists. Metagenomics requires rapid sequencing, yielding staggering amounts of genomic data that demand new computational approaches to exploit the wealth of information contained in the global genomic realm. Metagenomics can help in new ways to understand the relationship between genes and complex molecules like proteins and RNA, which for example can be used to exploit the genomic information of parasites and hosts to develop a novel class of antibiotics. These relationships may ultimately dictate the evolutionary processes that determine the structure, function and preservation of ecosystems, and are ultimately a significant determinant of the well-being of humans (one need look no further than the Gulf coast). ***The LI will provide the resources needed to make this initiative successful, which in turn will provide momentum for the upcoming Center for Integrative Microbial Biology at LSU.***

Ciliary Motion is a specific example of a biologically and physiologically significant area of investigation that incorporates multiscale analyses, fluid-structure interactions and biotransport, for which computational simulation provides a powerful tool for understanding complex coupled processes. In the human body, cilia and flagella are present on almost all cells. These hair-like appendages are central to ovum transport in the oviduct, transport of mucus across respiratory epithelia, and cerebrospinal fluid movement in the brain. In the pulmonary arena, impaired ciliary motion is related to serious health problems such as cystic fibrosis. SI Fauci (Tulane) leads computational fluid mechanics work related to ciliary transport. Further ***understanding of these biological processes will result from the ability to perform large-scale computational fluid dynamics simulations.***

Pulmonary Mechanics: Pulmonary airway reopening relies on multi-scale modeling, fluid-structure interactions, biotransport, cell mechanotransduction and cell signaling events. Multidisciplinary studies will result in an improved understanding of these coupled processes that may lead to the design of protective mechanical ventilation strategies for opening occluded pulmonary airways with minimal damage to sensitive tissue. Interdisciplinary studies rely on computational biofluid mechanics investigations to understand surfactant transport processes and fluid-structure interactions that damage the lung [25, 26] While Tulane's research in this area has identified likely damage stimuli, ***CSs methods will be necessary to extend the current studies to incorporate realistic biophysical properties and more realistic geometries.***

Computational Biofluid Mechanics (Tulane): Computational biofluid mechanics methodology developed at Tulane is now being broadly applied to the study of permeable membranes, blood flow, micro-organism motility and cell motion. Such methodology includes immersed-boundary methods, boundary element methods, projection methods, and the method of regularized stokeslets,

which require advanced numerical techniques and algorithms. ***Progress will require working with computational material science teams.***

DNA Based Detection (UL Lafayette): Methods for the rapid detection and quantification of small organisms in environmental samples have broad application in environmental monitoring, fisheries biology, detection of pest species and biosecurity. PI Neigel has pioneered the development of DNA-based methods for species-specific detection and quantification of small organisms in water samples. The goal now is to develop methods that can simultaneously assay hundreds or thousands of different species in mixtures. A key to success will be a design process that integrates sequence information, chemical kinetics of DNA detection, and experimental evaluations. ***Cyberinfrastructure and computing workflow tools are needed to aid the design of new assays and to produce working prototypes that can be field-tested.***

Phylogenomic Protein Identification (UL Lafayette): As the complete genomes of more species are sequenced we find that many encode proteins new to science. ***The deduction of function from structure is a central, unsolved problem in bioinformatics.*** We use sophisticated models of protein evolution and extensive databases of structure-function relationships to predict the functions of novel proteins (phylogenomics). The aim is to identify candidate proteins and begin their characterization by biochemical and molecular methods as well as functional assays. Our approach utilizes not only evolutionary relationships, but also detailed models of protein evolution. This work involves collaborations between UL Lafayette, LITE and, CCT.

Understanding the Infection Mechanism of HIV-1 (LA Tech): The HIV virus infects cells from the immune system of the body, mainly CD4+ T cells, but also monocytes and macrophages. ***A computational program has been initiated to simulate the HIV-1 strand R5 proteins effects on the infected cells, developing a simulation for the apoptotic pathway in HIV-1 infected cells,*** using our previous work on signalling pathways [27] as a starting point.

Computational Science: The scientific work described above requires computational algorithms and sophisticated tools to mine and manage data, ease development of complex simulation, improve visualization and enable scheduling to share computational, network, data, and visualization resources. Such tools, developed through different funded projects, are being deployed across LONI to create an advanced Cyberinfrastructure (CI) supporting the Louisiana research base and enabling researchers to take full advantage of LONI capabilities. The *LI* will help ensure that CSs efforts address scientific needs, providing close collaborations between computer and application scientists. Illustrative ongoing projects, that address the PITAC recommendations (Sec. A), include:

Cactus Toolkit for Multiscale Simulations (LSU, LA Tech, UL Lafayette): There are many multi-scale problems involving CFD and MD. Building on the success of the Cactus-Einstein Toolkit we are developing Cactus-based CFD and MD Toolkits. By researching and developing discipline-specific abstractions, we can create flexible, portable and extensible code, that can utilize remote steering, effectively coupling different interfaces, grid services, multiple data structures, in an open, modular programming framework environment. ***Such Cactus-based CFD and MD toolkits will support the scientific goals of the biologists and materials scientists,*** especially those attempting multi-physics, multi-scale computational problems and bring together researchers across the State.

SAGA (LSU): The ability to run multi-physics, multi-scale codes in any desired configuration (i.e. no tight binding of a software component to a given resource) in any CI environment is a very hard problem to solve. This task is being made possible by coupling scientific codes with the SAGA interface [28]. A set of Cactus thorns ***using SAGA libraries for operations needed by the computational biology and materials projects will be developed,*** as will SAGA adaptors for all LONI services including grid/HPC software (e.g., Globus, Condor, Stork etc.) as well all higher-level LONI services like HARC [29]. Widespread adaptor development activity will help make the scientific code truly grid-portable and resource-agnostic.

Distributed Data Management (LSU, LA Tech): The efficient management, retrieval, and mining of distributed, heterogeneous data is critical to all proposed multi-scale projects. A major objective is how to create the necessary tools and middleware to deal with low-level data handling issues, and thus enable the domain scientists to focus on their primary research problem. Kosar's NSF-funded PetaShare MRI project is providing management of low-level data handling issues for several projects using LONI. Key technologies will include data-aware storage systems and schedulers to transparently manage data resources and scheduling data tasks for the scientist. Data streaming routines will be optimized for use in LONI for remote visualization, code coupling, migration, and archiving services. ***Such data management research and development will be highly transformative, changing how scientists perform their research and rapidly facilitating sharing of experience, raw data, and results.***

Scheduling Services (LSU): The HARC [29] co-allocator is being deployed on LONI to provide enhanced scheduling services to support automated scheduling for co-allocated jobs, such as coupled CFD/MD simulations and coupled simulation-visualization processes.

Algorithms For Medical Data Integration, Mining, And Discovery (LA Tech, CCT): Growing barriers between clinical and basic research, along with the complexities in conducting clinical research, make it more difficult to translate new knowledge to the clinic and back again. The CCT plays a critical role in formulating computational approaches that can be used to ameliorate the problem, and with the Pennington Biomedical Research Center is preparing the State for a major NIH Institutional Clinical and Translational Science submission. ***LA Tech researchers are working on interoperable middleware and associated algorithms for medical data integration, mining, and discovery critical for biomedical applications.*** Specific research projects in progress are: (i) the development and validation of analytic data mining and decision-support software tools for biomedical and clinical image classification, diagnostic discovery, and clinical decision; (ii) development of autonomous computational protocols for domain knowledge from medical researchers in computing data models for metadata enhancement and data mining based decision support.

Personnel and Workplan for Research, Education, and Economic Development: We now discuss the workplan of the PIs, the recruitment and training of various new and existing faculty, computational scientists, students, and the programs we will use to build on the above scientific and computational work.

LI PIs. *LI* research, education, and ED activities will be initiated by the PIs, SIs, and LONI Management Council members, and their collaborations. During the first year, as Fellows, Associated Faculty, Computational Scientists, students, and corporate partners are added, these initial projects will be expanded, and new ones will be started.

LONI Fellows. Eighteen new faculty will be recruited to populate the distributed *LI* as LONI Fellows. These will be largely recruited during the first two years (Sec. B.4). An additional 6 faculty, funded fully by the member universities, will also be recruited, potentially extending the number of LONI Fellows to 24¹. All fellows will be fully funded by their universities after Year 5. Creating a world-class program requires senior leadership; we envision, and have budgeted, 2/3 of the LONI Fellows to be recruited as senior faculty.

LI Associated Faculty. An important component of *LI* is its "Associated Faculty Program", where existing faculty at all campuses will be supported to develop projects with *LI* staff in the targeted areas. We have budgeted for 28 *LI* Associated Faculty positions (4 per campus and 4 available to any institution in the State), which will provide a month of summer salary, *each year*. Support will be for one year, renewable to a second year. An additional 4 will be available each year for any campus, including medical centers and community colleges. In total, *LI* will be able to involve as many as 140 faculty in CSs projects over 5 years. Awards will be made on a competitive basis, with

¹Criteria to determine LONI Fellow membership will be determined by the PIs.

preference given to the selected areas of computation science, biology, and materials, as described in Sec. B.3. Junior and senior faculty will be eligible.

LI Computational Scientists. A crucial component of the *LI* is a strong contingent of advanced staff computational scientists. Modeled after similar positions in national labs, with organization and operation inspired by a highly successful program in Germany [30] the *LI* will recruit 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 (Sec. B.3), 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 with to develop applications that make use of LONI hardware and the staff.

Graduate Student Support. We will provide well-paid stipends to support graduate students in exciting projects in CSs, materials, and biology. 36 graduate students will be supported directly by this program; at least as many will be funded independently by research projects across the State that will leverage LONI and *LI*. *LI* will create a dozen *LI* graduate student fellowships, with duration of 2 years each. These stipends will be granted through a competitive process to promising graduate students in years 1, 3, and 5. The students (and their advisors) will be expected to become competitive for external support after 2 years; if external funding is not generated member sites will be expected to provide additional funding to extend these stipends to a total of 4 years for the duration of normal PhD studies. Excellence and ability to succeed in CSs will be the primary selection criteria, and achieving good representation of currently underrepresented groups among these students will also be a criterion in the selection process. Stipends will be awarded at \$25K/year per student. The projects will often, but not always, be associated with the projects described above.

Education, Outreach, and Training Programs. 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 tool-based workshops. Sec. B.4 shows expectations are to train 500 researchers by Y5, with 400 active users of LONI facilities.

We will carry out three major programs in education with high statewide impact; (i) Assess ways to infuse CSs deeply into the curriculum across the state, and to work with the BoR, and national organizations, such as NCSA and SDSC (see Dunning, Berman letters) to integrate LONI and national resources into the classrooms of all LONI campuses. (LSU is partnered with NCSA on its Track 1 proposal for a \$200M petascale facility, with plans to integrate LONI sites for research and educational purposes.) (ii) Build on LSU SI Sterling's CS class on HPC this spring [14], which uses innovative HD video technologies only possible over optical networks like LONI to include students at LA Tech, Arkansas, UNC, and Masaryk University (Czech), we will develop distributed classes (at least 4 per year), in multiple subjects, making them available at campuses across the state. Sterling's pilot project is drawing international attention; we believe it will lead to external

funding, change higher education in the State, and become a model for innovative education across the nation. (iii) Partnering with the Council on Competitiveness (Booher letter), with SI Speyrer we will develop programs to involve (LCTC) community colleges in CSs research projects and training, and place students in local industry (Sec. B.4).

We will encourage undergraduates to participate in *LI* research projects, and provide opportunities for summer internships at national labs and companies (see support letters). We will also seek NSF REU site program funding for undergraduate research. We will involve LA High Schools, and have already planned specific projects with high schools across the state maintaining Sony Playstation 3 units as LONI grid resources, running hurricane, storm surge, and gravitational wave simulations on the grid. These programs will be expanded through the *LI*.

Economic Development (ED). We will hire a full time ED officer (EDO) to run an aggressive ED program that will be a centerpiece of the *LI*. The EDO will work closely with LED, member sites' ED offices, and national organizations like the Council on Competitiveness (Booher letter), to create a regional/national competitiveness initiative to develop opportunities for students and faculty to join companies in internships, match companies to *LI* projects in CSs, and create a *LI* university-industry partnership program, driving creation of URICs. The EDO will emphasize partnerships with member sites, but we will also investigate *LI*-specific URICs as appropriate.

National Partner Sites. The *LI* will work with other national centers, as indicated by the letters of support. The institutions represented by these letters are the initial set of partners, but *LI* will continue to seek additional partnerships. The partnerships will vary in scope to match the joint interests of the *LI* and each partner, but general concepts that will be pursued are: (i) common infrastructure and interfaces, to allow users of the partners' hardware and software systems to easily move between centers; (ii) collaborative projects, where both *LI* and the partner are working in similar areas and multiple projects can benefit from joint work; and (iii) personnel exchanges, where *LI* faculty, staff, and students will be able to visit partner sites (and partner faculty, staff, and students will visit *LI* sites) for both short- and long-term visit, including summer internships for students. The PIs already have an excellent track record in this area; just this week 3 LSU students won research awards for work carried out with lab partners LBNL and ANL.

B.2 Project Impact

LI's activities will be harnessed for economic development (ED) for Louisiana, with university-industry cooperative research centers of excellence (URICs) flourishing in five years. One quarter of the in-depth CSs projects will be reserved for corporate partnerships, in Y1 we expect this commitment to lead to at least six university-industry research projects. *LI* expects to develop at least 24 university-industry joint research projects of significant depth within five years, and each of these projects will have the potential to lead to university-industry research centers of excellence (UIRC). *LI*'s ED program aims to have at least six significant new investments from major companies for UIRCs, more than a dozen grants from industry, and dozens of faculty and students involved in industry internships. Building on the success of, and helping to aggregate the many, current ED efforts of the partners, *LI* will catalyze LONI's ED potential and will have broad impact on the state's recovery efforts and its human and capital scientific infrastructure.

As part of the recent \$7.5M investment in LONI's 85 TFlops computational infrastructure expansion, the LONI Management Council, supported by Governor Blanco, has reserved a percentage of LONI's HPC capacity for industrial partnerships. To quote the Governor: *"These enhancements to LONI's computing power will make the network particularly attractive to the kinds of companies we need here to energize our state's high-tech economy. That's why we're leveraging the state's investment in LONI by reserving 10% of the grid's computational power for the creation and retention of high-tech jobs. Simply put, any business in the state able to connect to LONI can use access to the network as an inducement to recruit companies that would benefit from world-class*

computational capacity.”

Building the computational infrastructure of LONI is the first, most critical step in creating the foundation for current and future, proposed opportunities in computational research and ED. Connecting to LONI resources, however, is only a step towards leveraging LONI investments in order to enable and accelerate technology-driven ED in the state. The *LI* represents the third, essential step in creating a comprehensive LONI infrastructure – combining networking and hardware with *applications, support, training, and scientific expertise* – that will not only attract but also enable companies interested in partnering with Louisiana to leverage LONI resources.

A 2006 Council on Competitiveness study [31] provides an in-depth analysis of the strengths, weaknesses, and performance of existing industrial partnership programs at national supercomputing centers. The report notes that companies indicated that the most important aspects of their partnership with the centers were (i) access to HPC resources and (ii) access to CSs expertise. By creating the *LI*, Louisiana is positioned to be effectively responsive to the needs and requirements of companies seeking partnerships tied to CSs.

The ED program under *LI* will serve to further advance the achievements already realized through Vision 2020, small business incubation programs across the state, and other activities. While the potential for new patents and licenses of technology will be a natural outcome of the talented collection of faculty, research scientists and students in the *LI*, it will also be a directed goal of the *LI* ED program, expecting to leverage such outcomes to generate opportunities for the creation of new Louisiana companies and/or R&D partnerships with existing companies. *LI* anticipates that through its coordinated ED effort, opportunities for job creation and training in areas of research and industry related to high-performance computing will rapidly evolve, with measurable results by Y2.

The *LI* ED program will receive oversight and guidance for its development and growth from the LONI Management Council, the LED, the Council on Competitiveness and the proposed, national ED advisory board (Sec. B.3). Operationally, the program will be coordinated by an ED Officer (EDO), proposed in the *LI* budget. The EDO will be responsible for implementation the ED program, facilitating communication and coordination with members of the *LI* and companies of interest as well as managing established industrial relationships and tracking project deliverables and accomplishments under the program.

B.3 Management Plan

The *LI* will provide proactive, visionary leadership, and strong management, for all activities including education and training, development of research projects and proposals for research centers and corporate partnership programs. *LI* has an outstanding management team, with the highest scientific credentials and an excellent history of leadership and collaboration.

Proposed management process. The project will be led by PI Seidel, currently LONI Chief Scientist, who has extensive experience in running large scientific projects at an international level in the USA, Europe, and locally in Louisiana, where in the last three years he has built the CCT (housing 150 faculty, researchers and staff) and helped bring LONI to reality. Seidel received the prestigious 2006 IEEE Sidney Fernbach award in recognition of his leadership in collaborative scientific and computational research.

LI management will consist of a Leadership Committee (LC) and a Scientific Committee (SC) that coordinate through the LONI Management Council (MC). The LC will be comprised of University Administration PIs (Appendix 5), PI Seidel, and the LONI Executive Director. The LC will meet in person at least every three months, and will represent and liaise with campuses on strategic and operational topics such as staffing, strategic directions, and inter-institutional agreements. The LC will develop recommendations related to planning, resource allocation, and implementation

priorities and strategies to accomplish the scientific research, education, and economic development (ED) goals of *LI*. LC decisions will be made by broad consensus with input from the MC, SC, and the two advisory boards described below.

The SC, comprising Biology, Material, and Computer Science PIs (Appendix 5), will lead the scientific agenda of the *LI*. The full SC will meet in person every six months and more often via HD videoconference as needed. Separate, domain specific committees will be formed as needed. The SC will work with the LC on the appropriate mechanisms for faculty, research scientist, and student selection and training, and for scientific project organization to ensure that the research agenda of the *LI* is driving the institutes agenda. SC decisions will be made by broad consensus and with input from the advisory boards, the LC, and the MC.

Together, the LC and SC will expand and strengthen the MC's ability to lead the rapid growth in research, education, and ED activities and advancements that are expected through *LI*. Upon funding of *LI*, the operational details of LC and SC and the decision making processes of these committees will be quickly finalized through approval by the MC. LC and SC are anticipated to be functional, active committees by the fall of 2007.

Advisory boards. We will immediately assemble two national advisory boards, for CSs applications, and for ED. These boards will consist of national leaders, who will meet once per year with *LI* senior management, to provide advice, and track progress, and report both to the LA BoR and the *LI* LC. Board members will be chosen by the LC, in consultation with the BoR and LED, and will include prominent national leaders, such as national organization directors and members of the National Academies and Council on Competitiveness such as Suzy Tichenor (Council on Competitiveness), Mary Wheeler (Austin), Jack Dongarra (Tennessee), Larry Smarr (UCSD), Klaus Schulten (Illinois), Fran Berman (SDSC), Rick Stevens (ANL), and Tom West (NLR), as well as prominent scientists in companies such as Ravi Armilli (IBM), Javad Boroumand (Cisco), Claude Baudoin (Schlumberger), and Steven Wheat (Intel).

Selection and recruitment of *LI* faculty, staff and students. Faculty searches will be run by the partner campuses, coordinated by the appropriate University Administration co-PI. Each campus will maintain autonomy in running searches and making decisions, with specific target areas coordinated through the LC for maximum coherence and statewide impact; joint searches will increase recruiting power, interviews may involve other campuses, and joint appointments may be considered if appropriate. Searches will begin immediately with most new Faculty starting in Fall 2008.

Computational Scientists will be recruited immediately, with anticipated start dates in Fall, 2007. Advertisements, screening of candidates, and hiring recommendations will be made through the *LI* SC with final decisions made by member campuses who will host the scientists.

Competitive graduate student selection, evaluated by a committee, will be based on the strongest promise in the areas of CSs, materials, and biology, and suitability for placement in appropriate research groups. Student progress will be tracked, and help in finding suitable funding sources after *LI* fellowships end will be provided.

Selection of supported projects. An important aspect of the *LI* will be the CSs projects it supports, through competitively-awarded project support (staff computational scientists will be assigned 4-5 projects each per year) and Associated Faculty positions (which include summer salary). A formal allocation process, overseen by the SC, will evaluate proposed projects according to the following criteria: (i) scientific excellence; (ii) potential of the project to utilize LONI; (iii) involvement in existing *LI* projects; (iv) relevance to corporate partners, (iv) likelihood of obtaining federal funding; (v) likelihood of successfully using national facilities; (vi) independent resources brought to the project, including external and campus matching funding. *Project and Associated Faculty proposals will include specific, measurable milestones*, which will be evaluated and strictly tracked.

Roughly 25% of the projects, Associated Faculty, graduate students will be reserved for academic-industrial research partnerships, e.g. materials simulation of transport in porous media (e.g., with Proctor & Gamble), reservoir modeling (e.g., with Schlumberger), chemical reactor simulations (e.g., with Dow), transport of digital media over optical networks (e.g., with Cisco and Sony), distributed storage middleware development (e.g., with IBM), molecular dynamics simulations for biosensor design, nanomaterials studies, coastal remediation, are examples of areas where academic-corporate partnerships could leverage investments in IT infrastructure for simultaneously advancing research, education, and industry in Louisiana.

Recruitment and management of support personnel. A scientific coordinator 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. We will also recruit a full time ED officer (EDO), who will work with the *LI*, local campuses, LED, and the Council on Competitiveness (Booher letter) to run a corporate partnership program, recruit corporate partners, identify projects of interest, summer internships with corporate partners, develop corporate sabbatical programs, and create industry-university centers of excellence.

Operational Issues. Administrative offices for *LI* will be housed at LSU with other LONI staff, which will also host a visitor program, paid in part by BoR funds, and in part by CCT, where members of any project can visit to work with each other. Computational scientists, hosted by each institution, will meet at least biweekly to discuss projects, coordinate approaches, ensure common use of cyberinfrastructure, work with LONI staff, etc.

Semi-annual all hands meetings will include all PIs, SIs, LONI Fellows, Associated Faculty, LONI Computational Scientists and Graduate students, LONI staff, and other interested parties. Advisory board members will be invited.

A *LI* web site linked to the LONI pages will provide public information about *LI* projects, participants, etc, along with a secure, internal site for coordinated between the project partners, using shared calendaring, on-line discussion tools, etc. The site will serve two primary functions including (1) *LI* communication and (2) progress/activity documentation.

Economic Development. The EDO will coordinate *LI* ED efforts, working with member sites, LED, and nationally with the Council on Competitiveness pilot program with USC and Calit2 in California (see support letters). This fully leverage the infrastructure of LONI and and research capacity of the *LI*, to recruit new technology businesses to Louisiana, and to commercialize *LI*-developed technologies, working with technology startup companies.

B.4 Performance Measures and Objectives

We have defined numerous metrics for *LI* success, including hiring of researchers, starting statewide interdisciplinary research projects and obtaining national funding, developing corporate partnership programs and companies, ensuring interdisciplinary and multi-institutional collaboration, and creating new education programs. The *LI* management will closely monitor these measures, and take action as needed to ensure they are met or exceeded.

Personnel

Objective	Metric	Success Criteria
LONI Fellows	Full-time faculty hires (2/3 senior faculty, 1/3 junior faculty)	10 by EO Y1; 15 (total) by EOY2; 18 by EOY3; 6 additional faculty in other areas by Y5. Nucleation of 12 new multi-institutional research groups by Y3.
<i>LI</i> Associated Faculty	Summer support provided	28 per year in each year; over 100 total
Scientific Coordinator	Person hired	1 hire, fall Y1; new hire in 6 months if vacant
ED Coordinator	Person hired	1 hire, fall Y1; new hire in 6 months if vacant
<i>LI</i> graduate students	Graduate students funded by <i>LI</i>	12 in each two-year period; 36 total; all students externally funded before PhD
<i>LI</i> Computational Scientists	Staff hired	6 hired by fall Y1; new staff hired in 6 months if position(s) becomes vacant
Additional LONI fellows added	Number of additional faculty, additional disciplines	2 more faculty per site; additional application discipline of importance to State (coastal modeling, astrophysics, petroleum engineering) by EOY4
<i>LI</i> Growth of LONI to national status	Receive federal funding for additional staff	12 staff funded from federal sources by EOY5

Research

Objective	Metric	Success Criteria
LONI Computational Scientists	<i>LI</i> projects underway	12 new projects underway by EOY1; 18 new projects per year thereafter; 84 total; 25% projects permitted to be continued for new advances; 25% corporate
State faculty, staff, and student trained and using LONI infrastructure	Number of applications for time, projects using compute, data, network, and software services	All <i>LI</i> projects use LONI, 400 active users from State, 12 from each <i>LI</i> members, medical centers and community college system
National proposals	<i>LI</i> -funded faculty-led national agency proposals, submitted, funded	50% of <i>LI</i> projects lead to funding from outside the State (e.g., NSF, DOE, NIH) or industrial funding in Y2 and subsequent years; 2 additional submitted per year, per Fellow, starting in Y2, 100 total, 20 new projects funded total
Research computing project resources	Successful computational infrastructure/cycle applications	50% of projects lead to nationally-judged computational infrastructure awards in Y2 and subsequent years
Research publicity	Invited presentations and lectures outside LA	Each project leads to 2 per year starting in Y2; 160 total
Scientific & Engineering Results	Peer-reviewed conference and journal publications that acknowledge <i>LI</i> support	3 per LONI Fellow per year; 1 per Associated Faculty per year; over 150 total
National Computing Center	<i>LI</i> personnel successful	1 national federally-funded computing facility, funded with at least \$70M
<i>LI</i> research impact	New non- <i>LI</i> -funded faculty working with <i>LI</i>	6 per year starting in Y2

Economic Development

Objective	Metric	Success Criteria
Student internships with companies	Number	6 students place each year; 30 total (not all will be <i>LI</i> -funded)
Pilot program with Council on Competitiveness	Established	20 students at community college trained in CSs each year, 50 total placed in companies, 20 enter universities for continued study in CSs
Industrial partnerships	Partnerships in projects with industrial partner	25% of total projects; 20 partners in 5 years
Industry grants	Sponsored research from companies	30 by Y5
Centers of Excellence (UIRCs)	Number formed with multi-year duration	1 by EOY3, 3 by EOY4, 6 by EOY5, all industry-funded with at least 1 industry staff member on-site
Companies formed	Number of new companies	1 by EOY3, 3 by EOY4, 6 by EOY5

Collaboration

Objective	Metric	Success Criteria
Between computational scientists and biologists, materials	Joint papers and proposals	2 interdisciplinary papers (including preprints from a <i>LI</i> 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
Inter-university	Number of joint papers, proposals	2 papers, 1 proposal (including preprints from a <i>LI</i> preprint series) per group per year
Inter-university	New joint projects	30 new multi-university projects proposed to SC per year
National	Visits to national labs	6 students, 2 staff, and 12 faculty with visits to national labs per year, 4-6 each summer

Education & Training

Objective	Metric	Success Criteria
Statewide education	HD video courses offered	4 courses per year with students from 4 universities, and 20 total students per course receiving credit.
Statewide training	Number of training workshops, people trained	4 HPC & CSs workshops offered per year, 100 people trained each year, 500 total
High school education	Summer camps	2 per year
High school courses	Teachers offer <i>LI</i> -related material in courses	10 new per year starting in Y2

B.5 Sustainability

The *LI* activities are crafted both for long term sustainability beyond the funding period and to significantly grow in size, scientific coverage, and State impact. Initially focused on biology and materials application areas along with fundamental CSs most critical to the State's economic future, and will add additional faculty in other areas. *All six member universities are completely committed to LI, fully funding the 18 LONI Fellow faculty positions that will be catalyzed by this project after its completion.* These new faculty, dozens of new graduate students, and roughly 100 existing faculty trained in the use of advanced CSs will create a powerful sustaining force to recruit additional faculty and students, hundreds of IT-based research and ED projects, and hundreds of millions of dollars in new federal and corporate funds in IT-based research and education.

In total, *LI members commit over \$16M during the initial five-year startup phase, and this amount increases after the first five years as BoR funding ends and the 18 faculty are funded at 100%. Further, by this time we also expect additional commitments of LONI member universities, much higher levels of federal funding, and corporate partnerships, such as:*

Additional *LI* faculty commitments: As new faculty openings become available, the universities

are committed to hiring faculty who can take advantage of LONI services specifically, and modern cyberinfrastructure generally, in all disciplines. As appropriate, new *LI* faculty will be recruited, funded fully by the members, in all areas of science, engineering, humanities, and business. *The LI will make recruitment of strong faculty much easier, will provide these faculty with much stronger support to develop prominent research programs, and will enhance their collaborations with other computationally-oriented faculty, while connecting them to ED programs, across the State for still stronger programs.*

Major STC and ERC centers: With a coordinated and focused approach, the State will be able to use its strengths to bring in major center funding, to support the *LI* and national research centers. NSF's Science and Technology Centers (STC) program was established to "fund important basic research and education activities and to encourage technology transfer and innovative approaches to interdisciplinary problems," and its Engineering Research Center (ERC) programs has similar goals. The State is on the brink of competitiveness for such centers, increasingly based on CSs that will be dramatically strengthened by the *LI*.

National petascale computing facilities: NSF's new Office of Cyberinfrastructure (OCI) will invest \$1B in cyberinfrastructure over the period of this proposal. The *LI* will recruit and/or train hundreds of State researchers in modern cyberinfrastructure, making them competitive for using national facilities, and bringing new facilities to the State. Recent investments make the State competitive for major center funds; it is currently involved in strong proposals to join the TeraGrid (\$5M HPCOPS), to create a national petascale facility (\$70M Delta), and to participate in the national leadership computing facility (\$200M hardware proposal, led by Illinois). *Creation of the LI will make the State much more competitive for such opportunities, and will lead multi-institutional proposals to for such facilities.*

Alignment with federal agencies: As stressed in Sec. A, virtually all recent strategic reports of National Academies, agencies (NSF, DOE, DOD, NIH, NASA), and PITAC recommend strategic shifts and increases in funding priorities to support interdisciplinary CSs, emphasizing growth areas in computational biology and materials. *The LI is squarely aimed at positioning the State to be a leader in these areas.*

Educational programs: As federal agencies realign funding priorities, programs such as EP-SCOR, IGERT, and Broadening Participation in Computing (BPC) are growing, and are more focused on developing expertise in development and use of CSs across all disciplines. *The LI will lead highly-competitive multi-institutional proposals in these and other programs.* Such projects will have a transformative effect on the State.

Corporate partnerships and centers of excellence: Working with LED, federal agencies, and the Council on Competitiveness, the *LI* will aggressively develop programs for joint university-industry cooperation in numerous areas. Preliminary discussions with companies and agencies (support letters) include creation of university-industry research centers (UIRC), senior industry researcher sabbatical programs, and industry sponsored internships and student support programs. Similar programs in other states, e.g., Illinois, have generated hundreds of millions of dollars in direct investments. LONI has already played a significant role in new industry interest and activities (e.g., with Thyssen-Krupp, Boeing, Schlumberger, IBM, Cisco, Microsoft, Intel, Lucasfilm, Sony). *Creation of the LI will lead to specific and significant new investments in the State from companies like these and others, leading directly to the kind of IT-based ED that is clearly needed.*

In summary, *LI* sustainability and growth will be ensured by: (i) *recruiting dozens of new faculty and students* supported by *LI* member universities and their research groups; (ii) *training roughly 100 existing faculty, and supporting/creating at least 6 dozen CSs projects* across the State that will be competitive for federal funding, from individual grants to STC, ERC, and national computation centers; (iii) *creating a competitive environment to attract university-industry partnerships* and centers for direct ED payoffs for the State.

C Leveraging of Resources

As stressed throughout (especially Secs. A.2 and A.3) the *LI* builds directly on significant State investments. The Vision 2020 IT Initiative committed \$25M annually to Louisiana's research universities (all represented here), calling for the advancement of six key technology industries, including IT, micromanufacturing, biotech, and materials. Higher education, identified as a driver for ED, was charged with the implementation of plans for (i) developing technologies that create new companies, jobs, and wealth, and (ii) developing a highly trained workforce for the IT-intensive workplaces of the new century.

With these investments, the institutions aggressively built infrastructure, recruited leaders, and created centers of excellence. **LSU** created the CCT in 2003 through, which has become an internationally recognized center for interdisciplinary CSs and applications;. **UL Lafayette**, with local industry, built the \$27M LITE center, one of the world's most highly advanced 3D visualization facilities to work with every industry. **UL Lafayette** has also established CBIT (A.3), dedicated to helping private businesses use modern technologies. **UNO's** new Advanced Materials Research Institute (AMRI) has received over \$38 million in funding since its inception in 1996, leading to a proposed multi-institutional collaborative PhD program in materials; it has also forged highly productive collaborative CSs programs in bioinformatics. **SUBR** built a CAVE (invented by Cruz-Neira), and created the Center for Information Technology Innovation (CITI), focusing on technology with long-term economic benefits. Its degree programs in e-Business will create *LI* student ED projects. **LA Tech** expanded its molecular/nano-scale CSs faculty and facilities in its Institute for Micromanufacturing; its CENIT center has developed a sequence of interdisciplinary entrepreneurship courses; students have already accelerated the commercialization of research in biotech, IT and materials, and will further efforts in innovative product and business plan development and venture research with the *LI*. **Tulane's** Center for Computational Science (CCS), founded in 2002, is dedicated to the use of CSs to address scientific research in biofluid mechanics, biomolecular processes, turbulence, materials, and more, and has already attracted \$10.3M in funding.

Further advancing Louisiana's IT infrastructure (initiated in 2003 by LSU's Seidel and Allen, LONI Director McMahon, and LITE's Tierney [32],) **LA** joined the National LambdaRail (NLR), and Governor Blanco committed funding for LONI, both in 2004. Louisiana became one of the first states to deploy its own high-speed optical network connecting its major research universities to the NLR. With an additional \$7.5M, LONI will expand its supercomputing capacity to nearly 100 TFlops, with machines at all six *LI* sites, giving Louisiana researchers the most powerful distributed HPC infrastructure in the nation.

These activities have placed the State in a position to be competitive, for the first time, for very large federal programs in IT-related science and engineering. Recent proposals, totaling in excess of \$100M (e.g., LBRN, PetaShare, Delta, Petascale facility, CyberTools, HPCOPS, UCoMS, etc.) (Secs. A.2 and A.3), are fundamentally based on having LONI in-place. *All of these projects share a common vision, and would have been uncompetitive or impossible without LONI and the close cooperation and coordination between the member sites.*

We have now reached the point where such efforts can be dramatically enhanced in a statewide institute, coherently harnessing these strengths and helping the State reach a self-sustaining critical mass. The State still needs many more researchers and students in the areas of CSs, biology, and materials, who are able to combine these strengths if it is to attain national leadership at a level that significantly advances the State's economy. ***LI is aimed squarely at achieving this goal. It integrates and enhances Vision 2020 IT strengths, and LONI infrastructure, with a coordinated statewide effort that is much stronger than its individual parts. All member universities are firmly behind the LI, which is unusually well-aligned with State and campus priorities. It will strengthen all our universities; it will strengthen our State.***