Title of Cluster:
Computational Science — Advancing Research, Society and the Economy

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<th>Name</th>
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<tr>
<td>Sumanta Acharya</td>
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<td>Gerald Baumgartner</td>
<td>Computer Science</td>
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<td>Bin Chen</td>
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<td>Jim Chen</td>
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<td>Rudy Hirschheim</td>
<td>Information Systems and Decision Sciences</td>
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<td>Computer Science</td>
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<td>Electrical &amp; Computer Engineering</td>
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<td>Robert Lipton</td>
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<td>Marcia Newcomer</td>
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<td>Jorge Pullin</td>
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<td>Christopher White</td>
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Disciplinary Theme or Academic Area of the Cluster:
Interdisciplinary Computational Science

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\(^1\)This document is a slightly amended version of the original proposal with e.g. budget details and names of exemplary hires removed.
Executive Summary: Computation is revolutionizing research, education, and economic development at every level, in every discipline, and in every business. It is now known as the “third pillar” of science and engineering, standing equally alongside traditional approaches of theory and experiment. Additionally, it is transforming the fundamental approaches to emerging areas of academic research in the humanities, business, and the arts. A new discipline of “Computational Science” has emerged, becoming a central theme of numerous world-wide academic programs. Through the Vision 2020 and LONI initiatives, the State has built a strong foundation for academic research and economic development, on which LSU has provided statewide leadership to capitalize, through its Center for Computation & Technology (CCT). Computer Science (BASC), Mathematics (A&S), and ECE (Engineering) have partnered with CCT to recruit leading computational scientists, in three years creating a close-knit, well-known interdisciplinary computational science group with applications such as astrophysics, fluid dynamics, music, and coastal engineering.

Based on this strong foundation we propose a comprehensive computational sciences cluster (CoSciCl) to build one of the strongest and most visible groups in the country, on which many other efforts (e.g., biosciences, coastal science, physical sciences, engineering, arts and humanities) will all depend. This will better align LSU to compete for large federal funding opportunities from all national agencies, and provide one of the most important ingredients for sustained economic development: a talented IT-based workforce.

The plan aims to bring 8 top faculty to LSU, in overlapping areas central to the PITAC recommendations (algorithms & software, hardware, and data & sensor networks). CoSciCl has broad campus support, and deep support from units involved most directly (CS, Math, ECE, CCT). The CCT will commit at least four 50% faculty positions and will recruit a high profile deputy director in this area (100% CCT-funded). We believe the chance of recruiting major figures is high. CoSciCl will make LSU a leading national force in this critical area that underlies most modern research and economic development activities.

A successful cluster in computational sciences, important in its own right, is also critical to disciplines spanning academic and industrial research. Programs in coastal modeling, computational-engineering, -biology, -astrophysics, -humanities, etc, are under development at campuses across the world, but they all require a strong foundation in computational sciences. The CCT is supportive of all such initiatives at LSU, through explicit commitments to support faculty in other clusters, and through this core CoSciCl initiative. The CoSciCl will make all other proposals involving computation much more competitive. CoSciCl is fundamentally interdisciplinary, involving at least three colleges, and providing a common interactive and supportive venue (CCT). This has many advantages; perhaps the most important is the integration of related but disparate efforts in research and education. This CoSciCl initiative will catalyze a uniquely powerful computational science educational curriculum that brings together multiple colleges, and will be a core component of many other educational programs to be developed at LSU, from biology to engineering.

The CoSciCl aims to enhance the economic development potential of the region, leveraging the State’s Vision 2020 and LONI to attract the most talented possible workforce in IT research. Similar efforts, e.g., at NCSA at the University of Illinois, have generated more than $120M in corporate partnerships, $400M in grants, spawned numerous companies, and the web browser revolution, with an estimated trillion-dollar impact on the world economy. Fulfilling such economic development possibilities requires a strong faculty in computational sciences and proactive leadership and policies.

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2 Found in the Presidential Information Technology Advisory Committee’s 2005 report to President Bush.
Computational Science Cluster (CoSciCl) Initiative

1 Description and Rationale

In its 2005 report to President Bush, entitled “Computational Science: Ensuring America’s Competitiveness”, the Presidential Information Technology Advisory Committee (PITAC) 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. The PITAC believes that computational science is one of the most important technical fields of the 21st century because it is essential to advances throughout society.” This report, and numerous others from virtually all government research agencies, are creating a fundamental realignment of academic and industrial research activities. For example, the NSF has created a new ($182M FY07 budget) “Office of Cyberinfrastructure”, DOE has created a program called SCIDAC (“Scientific Discovery through Advanced Computing”), and similar initiatives have been developed in NASA, NOAA, NIH, ONR, and beyond. LSU is positioned to be a leader as such programs develop, and a strong effort in computational science – as this proposal aims to create – will ensure that LSU will be able to advance in its leadership role.

The challenges are numerous, deeply affecting all disciplines, and must be met if the nation is to remain competitive. For example, the report of the NSF’s 2006 Blue Ribbon Panel of Simulation-Based Engineering Science (SBES) states “For more than a decade, researchers and educators in engineering and science have agreed: the 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 and implementation of dynamic data-driven application systems. We must improve methods to quantify uncertainty and to model validation and verification. 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 that SBES requires. The payoffs for meeting these challenges are profound. We can expect dramatic advances on a broad front: medicine, materials science, homeland security, manufacturing, engineering design, and many others.” Without a strong effort in computational sciences, LSU will not able to meet such challenges.

The effort to decode the very basis of human life, commonly known as the human genome project (HGP), is an interesting case study. The HGP is arguably the most significant scientific breakthrough in the last fifty years and it owes its success as much to advances in computational science (algorithms and high-performance computing) as it does to high-throughput screening. It also illustrates the larger emerging trend: the ability to generate data is increasing exponentially, but the ability to manage, analyze and extract information from ever increasing amounts of data has fallen far behind. Large-scale data sets cannot be analyzed and understood in a reasonable time without computational models, data and text mining, visualizations, and other knowledge discovery tools. In general, computing is the basis that will advance biology in the 21st century, just as mathematics was the basis upon which the major advances in Physics took place in the 20th century. Advances in computational sciences are needed to realize this vision, which is widely recognized, by researchers, agencies, and commissions worldwide. In 1998 the first Nobel Prize that relied on work in computational science was awarded to Kohn and Pople for devising a

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computational method that forms the basis of nearly all modern material science, including
the trillion dollar semi-conductor industry. This Nobel Prize, and others since, serve to
underscore both the importance of computational science as well as the path ahead.
The PITAC report singles out three areas of computational science that are critical to the
future of all research and industrial activities, recommending that “the Federal government
must rebalance R&D investments to:

- Create a new generation of well-engineered, scalable, easy-to-use software suitable for
  computational science that can reduce the complexity and time to solution for today’s
  challenging scientific applications and can create accurate models and simulations that
  answer new questions;
- Design, prototype, and evaluate new hardware architectures that can deliver larger frac-
  tions of peak hardware performance on key applications;
- Focus on sensor- and data-intensive computational science applications in light of the
  explosive growth of data.”

These research areas are fundamental to the emerging discipline of computational science.
Computational science is a wide discipline, as it combines both hardware and software
technologies, from the underlying devices that make up CPUs, on which all the software
runs, to the operating systems and run time systems that are common to the hardware, to
the middleware (databases, communications and mathematics libraries, sensor interfaces),
to the domain specific frameworks themselves. Simulations and models can then be built
on the computational science foundation built from the combination of all these elements.
Progress in this new “third pillar” of scientific discovery, which complements theory and
experiment, requires experts who specialize in these topics, but who work closely with sci-
entists, engineers, and scholars in humanities and other traditional disciplines. Building on
recent progress at LSU, and on statewide investments in IT (e.g., Vision 2020, LONI,
etc.), supporting the LSU Flagship Agenda we propose a coherent “Computational
Sciences Cluster” (CoSciCl) that will:

- Bring LSU to international prominence in this critical emerging discipline for the fu-
  ture, addressing all three areas emphasized by PITAC;
- Create strategic alignment of LSU with major research funding agencies for decades;
- Support and strengthen many other initiatives across campus, resonating with many
  other cluster hire proposals;
- Have economic development impact in areas where the state is heavily investing;
- Build on the interdisciplinary partnerships created over the last few years joining col-
  leges of Arts and Sciences, Basic Sciences, Engineering with the CCT.

To achieve these goals, we will recruit top faculty with proven history of leadership in
interdisciplinary computational sciences, or with clear potential to do so. This is discussed
in detail in §2.

1.1 Special Role of the CCT in the CoSciCl and other Cluster hires

Although this proposal is driven by faculty from multiple departments at LSU, the CCT
plays a special role in catalyzing computational science development and integrating it with
units across campus. CCT is an interdisciplinary research center focused on computational
science and its applications. It creates joint, 50-50 faculty appointments with departments
in virtually all colleges, (currently, CCT faculty span 12 departments), seeking to advance
LSU’s mission in research, education, and economic development. CCT directly addresses a principal recommendation of PITAC, which warns “Among the obstacles to progress are rigid disciplinary silos in academia … These silos stifle the development of multidisciplinary research and educational approaches essential to computational science. Our report recommends that both universities and Federal R&D agencies must fundamentally change these organizational structures to promote and reward collaborative research.”

In partnership with LSU’s colleges, in just three years, CCT it has made great progress in creating a new structure to address problems inherent to multidisciplinary research. It has developed four interlinked “Focus Areas” of research and education: the “Core Computational Sciences” (CCS) Focus Area, fundamental to this proposal, as well the application-oriented Focus Areas in “Coast-to-Cosmos”, “Material World”, and “Human and Social World”. In addition to office space in their home departments, all researchers also have office space in a shared, common environment in the CCT as well, and are encouraged not only to work together, but also to help advance the computing environment. To quote Jim Pool, formerly Executive Director of Caltech’s Center for Advanced Computational Research, “It is my impression that CCT has the best opportunity among all the academic sites to develop into a center with a major research agenda. Other academic sites have seem to have either a facility orientation or a struggling research program. In the last decade, places like Princeton, Harvard, Chicago, … have tried and not succeeded. Remarkably, LSU has gotten farther than any of these places in a very short period.”

This CoSciCl proposal builds out the CCS Focus Area, strengthening participating departments, while providing a collaborative venue and incentives for them to work collectively. At the same time, it provides them with direct interconnections with the application areas, which connect to still more units across campus. The faculty have developed a “Faculty Plan” which outlines specific strategic areas to be developed in all focus areas. This Faculty Plan effective argues for a number areas of concentration that can be built on the computational sciences. In concert with this “grand plan”, CCT is also highly supportive of other cluster hire proposals in the following areas, which naturally resonate with its goals, and would effectively bring this plan to fruition: Materials, Digital Media, Astrophysics, Polymer Science, Propulsion, Coastal Sciences, Computational Biology, Porous Media, and Computational Electronics. Each of these has a computational component that is greatly strengthened by this CoSciCl proposal; in fact, we argue that a strong CoSciCl cluster is necessary for the others to fulfill their promise. Conversely, the CoSciCl proposal is strengthened by each of these. Many of these proposals contain faculty areas or even specific candidates that overlap with areas proposed in CoSciCl.

The timing is excellent for this proposal. It has taken three years to arrive at this turning point (see next section) where we can launch such a bold initiative and be confident of success. Earlier, it would have been premature, and at the same time, in three more years it may be too late; other universities will seize the lead if we do not.

1.2 Building a Future on Current Strengths in Computational Science at LSU

Current State: In three years, LSU has developed strong computational science faculty in CCT’s CCS Focus Area in Physics, CS, Math, and ECE, adding three Gordon Bell Prize winners (Allen, Seidel, and Sterling), a 2006 Sidney Fernbach Award (IEEE) and Heinz-Billing Prize (Germany) winner (Seidel), an NSF Young Investigator Award winner (Ramanujam), and numerous winners of HPC and best paper awards at SC and other con-
ferences (Allen, Jha, Katz, Ramanujam, Seidel, Sterling), among others. (These are among the most prestigious awards in the discipline.) The faculty have also generated millions of dollars in federal and state funding, creating strong interdisciplinary projects in coastal modeling, astrophysics, fluid dynamics, and petroleum engineering, grid computing, and visualization, to name a few. The broad research interests of current faculty cover:

- Application tools and frameworks (Gabrielle Allen (CS), Ian Taylor (CS, joint with Cardiff), Ed Seidel (Physics/CS))
- Data and grids (Tevfik Kosar (CS))
- Computer architectures (Thomas Sterling (CS))
- Networks (Seung-Jong Park (CS))
- Performance (J. Ramanujam (ECE))
- Finite elements and multigrid (Susanne Brenner (Math))
- Linear algebra (Paul Saylor (Math, visiting from Illinois))
- Multiscale algorithms (Burak Aksoylu (Math))
- Scientific computing (Daniel S. Katz (ECE))
- Visualization and interaction (Brygg Ullmer (CS))

Future Growth: This is a strong start, but the group needs to grow in particular areas if it is to provide the comprehensive foundation needed to address the needs of campus. With additional strong recruits as proposed, our faculty can create one of the most powerful, comprehensive efforts worldwide. Areas of top priority are: compilers and operating systems, visualization, programming languages, scientific computing, linear and hyperbolic equations, and large scale computing systems. The CCT is sufficiently advanced in CCS that it should be very competitive for recruiting some of the top people in these fields, forming the foundation on which to build the application clusters discussed in other cluster proposals, and in the CCT Faculty Plan, which is fully aligned with the Flagship Agenda.

While this cluster starts with four or five units involved, it spans multiple colleges as well as one center. Success with this base will lead to involvement of other departments within these colleges, as well as involvement of additional colleges over time. CCT already includes faculty from 12 departments, showing that computational science has the potential for rapid expansion throughout LSU. As we have argued above, the CoSciCl initiative will strengthen other computationally oriented clusters, further enabling them to grow as well.

As funding agencies follow PITAC’s recommendations, they are creating many interdisciplinary programs—with large funding streams—that actually require a strong coupling of computational scientists and discipline scientists. Such programs typically fund postdocs and graduate students to work together, creating more growth opportunities. We expect CoSciCl to help create a sustainable growth path for the entire university community.

Enhancing our Reputation and National Ranking: Primarily through CCT and Acharya’s IGERT program, LSU has already begun to have a national reputation in computational science, as demonstrated by Pool’s quote above and from this email from Horst Simon, director of DOE’s Berkeley NERSC, who commented on our recent joint proposal to NSF for a $70M supercomputing facility “congratulations. I think that this is a solid proposal with a great platform solution and a credible approach to build a new center. You are responsive to what (I think) NSF wants, and you were leading a great team effort...even in case NSF decides to fund another proposal, you have already established LSU as a credible contender on the national HPC scene, with good chances in future competitions.”
The recent recruitments of Professors Allen, Brenner, Katz, Seidel, and Sterling, and the visiting appointment of Paul Saylor (Illinois), have all attracted significant international attention and visibility in computational sciences in a very short time, making it much more likely to succeed in recruiting additional leaders through this CoSciCl proposal. **We are confident that CoSciCl will allow LSU to leapfrog many other universities in these areas, catapulting it to the upper echelons of computational sciences, dramatically improving its rank in multiple departments.**

It is very important to stress that CoSciCl is important not only in its own right, but that it will tremendously strengthen LSU’s competitiveness in many other disciplines. Not only will existing LSU faculty be able to develop novel and more powerful approaches to their current research activities that will give them an edge over the competitors, national leaders in computational approaches to biology, chemistry, physics, engineering, coastal sciences, social sciences, humanities, and others will be find LSU a more compelling and attractive environment to work, improving our ability to recruit them.

**Commitment of the Constituent Units:** The units are completely committed to the CoSciCl. The CCT has committed to jointly fund at least 4 joint positions at a senior level, specifically in the areas of Scientific Computing and Computational Mathematics. The departments of Math, CS, and ECE have developed a strong partnership with CCT in this area, and are committed to recruiting these and other top faculty in the areas described.

### 1.3 Potential for Success

There is a very high potential that this cluster will be successful, as the constituent units are committed to this plan and they have already shown their dedication to both interdisciplinary research and computational science within their disciplines. One example of this is CCT’s faculty plan, which builds on the interdisciplinary nature of the center and calls for additional faculty to expand the Governors’ IT mission. While other universities have already developed computational science programs, LSU’s is already strong, with unique advantages, such as the CCT, that are very attractive to prospective faculty.

Because of this, LSU has managed to recruit internationally respected faculty in the last three years in computational sciences. At the same time, it has been approached by, or initiated serious discussions with, international figures. We are confident that if our CoSciCl proposal is approved, we are likely to be able to successfully recruit some of these and other top figures that will both take this effort to the highest levels, while attracting still other faculty in other areas (e.g., biology, propulsion, digital media, astrophysics, etc).

### 1.4 A Unique Initiative with National and International Resonance

It should be clear that CoSciCl resonates nationally and internationally with other efforts at universities and national labs, as well as with new strategic directions of funding agencies in the US. It also resonates with funding streams in the EU and in Asia (some of the PIs have led international efforts funded by US and EU agencies.)

Many universities and US labs are developing groups in computational science, but only a few have depth in all areas recommended by the PITAC report (notably, e.g., Illinois, UCSD, and UT-Austin at the university level; ANL, NERSC, and ORNL at the national lab level). These sites, among others, have developed very strong academic programs around them, that fan out into all disciplines. ORNL and ANL have recently partnered with the Universities of Tennessee and Chicago respectively to create centers of excellence in science, engineering, and the humanities, that leverage these strengths in core computational
sciences. Such efforts are analogous to various cluster proposals we are involved in at LSU, e.g., biology, propulsion, materials, astrophysics, digital media, etc. Without a strong foundation in computational sciences, such efforts will struggle. As the remark from Jim Pool of Caltech above makes clear, our CoSciCl proposal is unique nationally in two critical ways: (i) this comprehensive program it is centrally housed through CCT, uniting efforts in multiple colleges, and (ii) it is connected tightly to other clusters in application areas.

1.5 Impact on Economy, Environment and Culture

Computational science has been identified as crucial for the Nation’s leadership and economic competitive in many reports, from PITAC, the Council of Competitiveness, and various Blue Ribbon panels. This message is also recognized in Louisiana, and led to initiatives such as Vision 2020, the CCT, and LONI, all of which are seen as major long term investments in making the state more competitive economically. The CoSciCl will allow LSU to recruit many talented faculty, staff, postdocs, and students with expertise in computational sciences. According to PITAC, “In the marketplace, computational science provides a competitive edge by transforming business and engineering practices. Integrated modeling and simulation techniques enabled the Boeing Company to minimize wind tunnel testing...resulting in cost savings and reduced time to market. In a recent Council on Competitiveness survey of businesses, the overwhelming majority said computational science was not only beneficial but also essential to company survival. [However, a] dearth of qualified computational scientists was a significant impediment to broader commercial deployment of computational science tools, techniques, and infrastructure. Researchers at national laboratories and universities have echoed this concern, noting the difficulty in finding graduate students, post-doctoral research associates, and staff members with the range of disciplinary and computational skills needed. Of the declining number of U.S. students...computational scientists represent only a tiny fraction.”

Addressing these issues, the CCT, which was founded on the premise that computational science is critical to statewide economic development, will work with other units at LSU to develop the CoSciCl into an economic engine, partnering its faculty, staff, and students with companies in the state and across the country to enhance their competitiveness through computational science. It has specific economic development milestones in its strategic plan, and programs to encourage its faculty and staff to work with companies and agencies across the state. It has staff specifically tasked with developing this mission, and will work to strengthen economic development programs in conjunction with the CoSciCl and other clusters it is associated with.

Going beyond partnering with existing companies, CoSciCl and related activities will create a strong base of talent in the area, making it much more attractive for companies to locate in Louisiana. CCT alone has already attracted roughly 100 skilled researchers in the last 3 years. To quote Carly Fiorina, former CEO of HP, “When we make a decision about where to locate a Hewlett-Packard facility, we have one criterion in mind. We go where the highly skilled and creative people are.”

1.6 Enhancing Doctoral and Undergraduate Education

Educational programs in computational sciences are struggling to develop, and are badly needed. To quote PITAC: “The number of graduates from computational science programs is inadequate to meet even current demand, and it is far below the number that will be needed in the future. This demand exists both in national laboratories and universities and in commercial contexts, as shown by the Council on Competitiveness. It is past time for
universities to take action. They must examine their educational practices and organizational structures to provide and reward interdisciplinary and collaborative research and education. New structures, programs, and institutional incentives are urgently required.”

CoSciCl will address this head-on, developing a coherent computational sciences educational curriculum for both graduates and undergraduates, spanning multiple colleges, building on the strengths already developed through the CCS focus area with faculty in CS, Math, and ECE. Computational science applications present a different approach to learning, based on problem-solving, computational techniques, and collaborative culture. The CCT already houses a new interdisciplinary IGERT program in computational fluid dynamics, and is already beginning planning for an inter-college curriculum in computational sciences. CoSciCl will enable LSU to create a uniquely strong program, compared to peers nationwide, in this critical area.

Funding agencies are also recognizing the critical importance of computational science education. In addition to NSF’s IGERT program, it recently launched CPATH⁶ – CISE Pathways to Revitalized Undergraduate Computing Education – a new program aimed at transforming undergraduate computing education on a national scale. The goals of CPATH are ambitious, challenging those who are in the best position to bring about real change. It is structured to stimulate broad conversations about the future of computing education, recognize and develop leaders, support the evaluation of the effectiveness of innovative approaches, and result in the propagation of the best models and practices. CPATH is focused both on the education of computing professionals and on the preparation of a broader professional workforce fully capable of utilizing computing technology in a wide range of application domains. In conjunction with the existing strengths outlines above, the CoSciCl will firmly place LSU in the rarified ranks of a handful of institutions that will be able to steer the national agenda in Computing Education with significant impact within the State.

2 Proposed Cluster Hires

We plan to recruit top faculty with a proven history of leadership in interdisciplinary computational sciences, or with clear potential to do so. We anticipate that many or all of the recruits will have broad interests, so that they will have primary and adjunct appointments, increasing interdisciplinary interaction between colleges. A full list of the example hires for this cluster was provided in the original proposal, the table below shows potential areas for each hire. We anticipate making senior hires first, as early as 2007, to aid in attracting the best of the new generation of computational scientists as junior hires.

Not in this table is the position of CCT Deputy Director, which CCT expects to fund and recruit this academic year. We expect this person to be a nationally known figure in high performance computing, who may also wish to have a faculty appointment in one of the departments listed. When filled, this position will add to the strength of CoSciCl.

⁶http://tinyurl.com/3daxtb
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<td>1  Scientific computing</td>
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<td>2  Scientific computing, runtime support</td>
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<td>3  Operating systems, compilers, runtime systems</td>
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<td>4  Linear systems</td>
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<td>5  Scientific visualization/ graphics</td>
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<td>6  Hyperbolic PDEs &amp; AMR</td>
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<td>7  Data middleware</td>
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<td>8  Sensors</td>
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While it will not be easy to get key figures to move, initial discussions with some leaders in these fields have led us to believe that LSU would be very competitive, both for reasons unique to each person, and for the one common reason that when we describe the computational science work that has been started at LSU, their voices become more animated as they consider the part they might be able to play, working with others at the same level, in creating the best example of integrated, multidisciplinary computational science in the world. Institutional support for computational science through cluster hires in this area will possibly provide just the boost required in efforts to bring these distinguished luminaries to LSU.