LSU's
Center for Computation & Technology
(CCT)

Joel E. Tohline, Director

CCT is …

An LSU research center whose mission, in part, is to infuse and enable computation – especially at the high end – into the forefront research and creative activities of all disciplines.

- Faculty lines – currently, 26 (avg. 50/50 split appointments) across 11 departments and 6 colleges/schools; tenure resides in home department
- Cyber-Infrastructure – guide LSU's (and state's via LONI) cyber-infrastructure design to support research ➔ high-performance computing (HPC), networking, data storage/management, & to some extent, visualization; also associated HPC support staff
- Enablement staff – currently 12 senior research scientists (non-tenured; ideally, on soft money support) with HPC expertise who support a broad range of compute-intensive research projects
- Economic development – to date, most significant interactions have been with Louisiana's burgeoning digital media industry (e.g., video game design; visual effects)
- Education – Influence design and content of interdisciplinary curricula; for example: (1) computational sciences, (2) visualization, and (3) digital media

Brief Historical Perspective

PART 1

Information Technology@LSU

New Faculty Positions in Multiple Areas

This year, through Governor M. J. "Mike" Foster Jr.'s leadership, the Louisiana legislature approved $22 million in new, recurring funding for a statewide Information Technology (I.T.) initiative to build research capacity and promote economic development and diversification throughout the state. Governor Foster proposed this initiative to complement Vision 20/20, the state's master plan for economic development, which calls for advancement in six key technology areas (www.lded.state.la.us/new/vision2020/centers.html). Higher education has been identified as the driver for economic development in the I.T. areas and, as the state's flagship institution, Louisiana State University (LSU) has been charged with a leadership role, receiving $7 million in recurring funds in the current budget year, to rise to more than $9 million on July 1, 2002. LSU is working closely with four sister institutions—Louisiana Tech, the University of Louisiana at Lafayette, the University of New Orleans, and Southern University—that are also targeted for investment under the governor's initiative.

In connection with this initiative, LSU has established a Center for Applied Information Technology & Learning (LSU CAPITAL). The objectives of this center are

- to better prepare LSU students to enter the modern, I.T.-intensive workplace;
- to focus more of LSU's research enterprises on I.T.-related fields of discovery; and
- to promote a more rapid deployment of new technologies into the marketplace.

LSU CAPITAL will provide the framework and infrastructure necessary to foster vibrant interactions among all faculty engaged in information technology research and teaching. New faculty, including some who will be appointed to endowed chairs and professorships, will be hired into several new "cluster" areas with the following research foci: core computing and communications, biological computing, materials science and engineering, and information systems. Efforts are under way to enhance the University's high-performance computing and communications infrastructure through the acquisition, for example, of a teraflop-class Linux cluster supercomputer. By 2006 between three and four dozen high-quality faculty hires will be made through LSU CAPITAL, beginning with the 2002-03 academic year.

Director of LSU CAPITAL

LSU is seeking applications for a permanent director of LSU CAPITAL. The successful candidate must have a Ph.D. and an established record of exceptional research and teaching in a subfield of information technology, such as one of the areas mentioned above. The director must understand how to interface well with the state's business community and how to transfer to the marketplace discoveries that are made through research in an academic environment. The director must have the ability to manage people within a large program; extremely strong organizational and communication skills; sound judgment; a desire to innovate; and a strong work ethic. Reporting to the Provost through the Vice Chancellor for Research, the director of LSU CAPITAL will lead efforts to hire exceptionally qualified faculty into new I.T. clusters, as described below, and will partner with the Vice Chancellor for Research in spearheading efforts to promote an entrepreneurial atmosphere throughout LSU's research enterprise.

Core Information Technologies

LSU seeks to hire outstanding tenure-track faculty with research and teaching expertise in the core areas of information technology. These include both theoretical and application aspects of, for example, high-performance computing; networking and tether-free communication systems; advanced data mining, storage, encryption, handling, and/or visualization; and the human-computer interface. LSU expects to make both junior and senior appointments in this area and will consider hiring an appropriately configured interdisciplinary group should the opportunity arise. The "core I.T." faculty cluster will sit at the center of LSU CAPITAL, providing transdisciplinary expertise to researchers in other I.T. clusters, such as those described below. In this spirit, selected faculty will hold joint appointments within LSU CAPITAL and one or more academic departments, as appropriate. These appointments may be through the Departments of Biological Sciences, Chemistry, Civil & Environmental Engineering, Computer Science, Electrical & Computer Engineering, Industrial & Manufacturing Systems Engineering, Information Systems & Decision Sciences, Mathematics, Mechanical Engineering, and others.

Biological Computing

Advances in transdisciplinary, I.T.-based research will profoundly influence the future of the biological sciences. LSU CAPITAL seeks to strengthen ongoing interdisciplinary efforts in biological computing and visualization by hiring outstanding tenure-track faculty with the mathematical and/or computational skills needed to advance genomics/bioinformatics at the genetic and evolutionary scale, and to advance physiological understanding of cellular signal transduction mechanisms at the cellular and molecular level, including macromolecular structure and interactions. Drug and vaccine design, biomaterials development, biosensors and intelligent biodiagnostics, and new algorithms to advance the interpretation of genomic/proteomic information are among areas of interest.

Materials Science & Engineering

New discoveries and applications in materials design and technology have been essential components of the rapid advances in electronics and biomedical and information technology driving the modern economy. In particular, the design and characterization of new materials provides for the development of smaller, faster, and higher performance components. Understanding of materials properties enables more effective means of developing processing techniques in the I.T. areas. We are seeking exceptional faculty whose scholarly interests will enhance and deliver additional technological advances. These joint appointments will be made between LSU CAPITAL and appropriate academic units, including the biological sciences, chemical engineering, chemistry, civil engineering, computer science, electrical and computer engineering, mathematics, mechanical engineering, physics and astronomy, and others. Initial hires will augment interdisciplinary strengths in microelectromechanical systems and nanostructured materials. Expertise in micro/nanoscaled materials, macromolecular studies, advanced fabrication techniques, and designed processing will facilitate microdevice research. Research in materials design, modeling and simulation, and engineering—including work on dual phase microcomposites, superconductors, and processing materials to create novel microdevices for biological, environmental, medical, and sensing/actuation applications—are of particular interest.

Information Systems

Advances in computing hardware, software, telecommunications, and related services have spawned fundamental changes in the marketplace and in the very nature of competition itself. Within a given business enterprise, the impact of information technology upon business processes and practices has been pervasive.

LSU CAPITAL seeks faculty to augment ongoing research efforts that focus on the efficient deployment and use of information systems in organizations, as well as the ways in which advances in information technology, particularly the Internet and electronic commerce, are creating sweeping changes in the way people live and work. Through these positions we expect to strengthen the interdepartmental information systems program in the E. J. Ourso College of Business Administration and develop a strong synergy between this program and other core areas of I.T. research, such as computer science, computer engineering, industrial engineering, and mathematics. We expect to make appointments at all levels of tenure-track faculty, including three endowed chairs and a number of endowed professorships, in a variety of fields, including information technology strategy, management of technology, enterprise resource planning, supply chain management, knowledge management and information retrieval, financial information systems, electronic commerce, and collaborative technologies and virtual teamwork.

The University

LSU is classified as a Doctoral/Research-Extensive University by the Carnegie Foundation, and is also one of only 25 universities nationwide designated as both a land-grant and a sea-grant university. LSU is the flagship research university in Louisiana's public system of post-secondary education. LSU currently (fall 2001) enrolls more than 31,000 students. In 2000–2001, LSU awarded more than 5,300 degrees, including more than 4,000 bachelor's degrees, nearly 1,000 master's degrees, 164 doctorates (Ph.D. and Doctor of Musical Arts), and 79 doctorates in veterinary medicine. Baton Rouge, located on the Mississippi River 70 miles north of New Orleans, is the state capital and the geographical center of South Louisiana's famed cultural, historical, and recreational attractions.

LSU is moving quickly with high levels of focus to advance in key areas. On the undergraduate level, LSU has transformed what was an open admissions university only 13 years ago into an increasingly selective institution. In 1988 the six-year graduation rate was 39 percent; it is currently 58 percent, having just recorded a rise of four percentage points over the previous year. LSU is implementing a residential college system for its undergraduates, including a new I.T.-immersive residential college that will open in fall 2002.

On the graduate level, LSU offers nationally competitive programs across the full disciplinary spectrum of the sciences, social sciences, arts, and humanities. The University has identified 12 programs as its "foundations of excellence"—and has allocated some $10 million to those priority programs in the last three years. Typical among the "foundations of excellence" is the Department of Chemistry that has for several years been the nation's leading producer of African American Ph.D.s in chemistry and that, according to the October 29 issue of *Chemical and Engineering News*, ranked eighth in the nation in 1999 among all universities, private and public, in expenditures on chemical research equipment. Other "foundations of excellence" programs of central importance to the research foci of the information technology initiative are in information systems and decision sciences, chemical engineering, biological sciences, mathematics, and physics and astronomy. LSU also boasts a variety of exceptional research facilities, including a synchrotron light source (the Center for Advanced Microstructures & Devices) that supports research in materials science and engineering and in the biological sciences (for example, with a beamline dedicated to protein crystallography). Learn more about LSU at the University's website, www.lsu.edu.

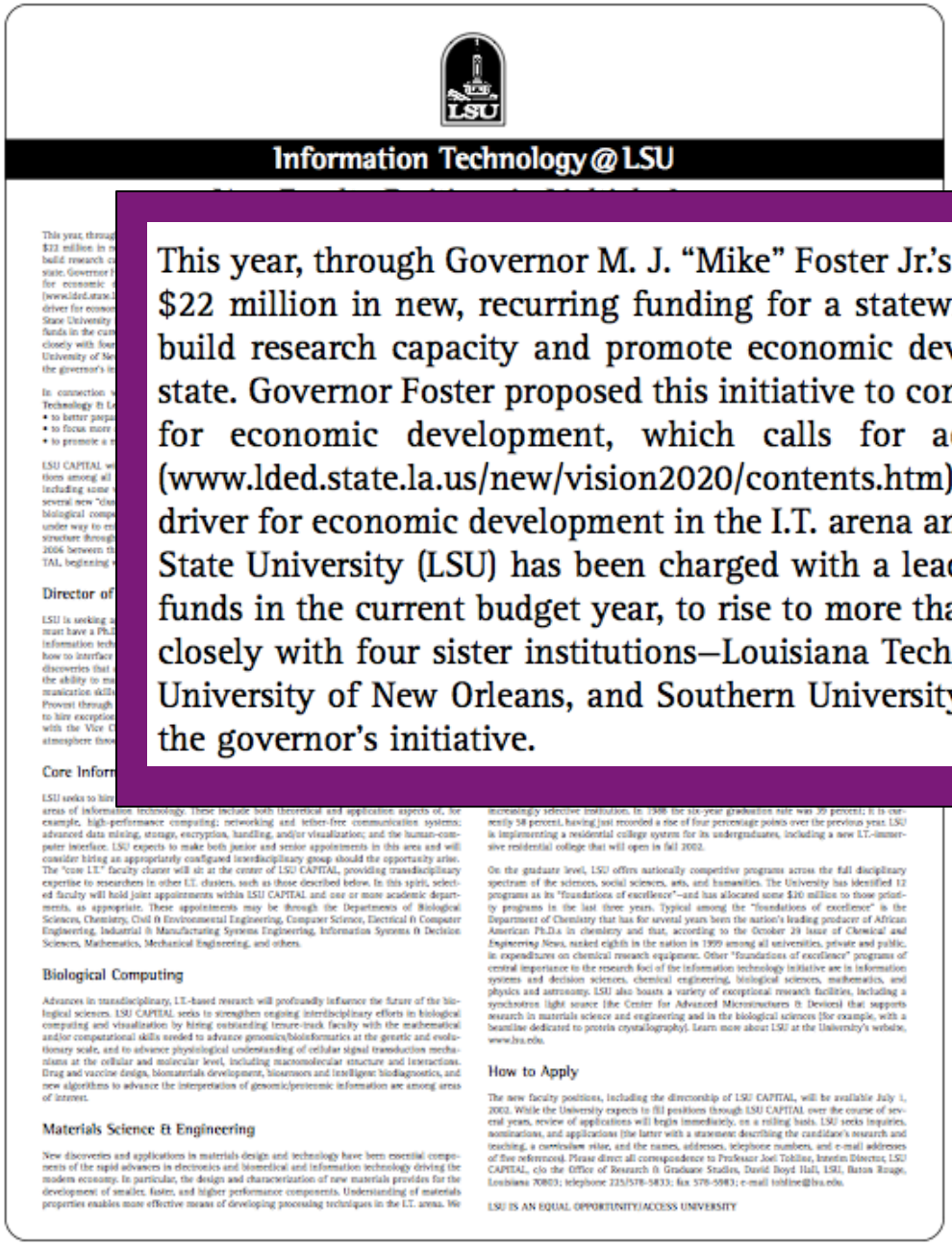
How to Apply

The new faculty positions, including the directorship of LSU CAPITAL, will be available July 1, 2002. While the University expects to fill positions through LSU CAPITAL over the course of several years, review of applications will begin immediately, on a rolling basis. LSU seeks inquiries, nominations, and applications (the latter with a statement describing the candidate's research and teaching, a curriculum vitae, and the names, addresses, telephone numbers, and e-mail addresses of five references). Please direct all correspondence to Professor Joel Tohline, Interim Director, LSU CAPITAL, c/o the Office of Research & Graduate Studies, David Boyd Hall, LSU, Baton Rouge, Louisiana 70803; telephone 225/578-5833; fax 578-5983; e-mail tohline@lsu.edu.

LSU IS AN EQUAL OPPORTUNITY/ACCESS UNIVERSITY

Year: 2001

Year: 2001



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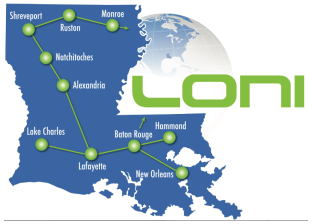


Year: 2004

Governor Kathleen Blanco announces that the State is committing $40 million to the Louisiana Optical Network Initiative (**LONI**) over the next 10 years.

VIEW FROM CAMPUS LAKE & WEST LAKESHORE DRIVE WITH ORIGINAL LETC I BUILDING AT LEFT

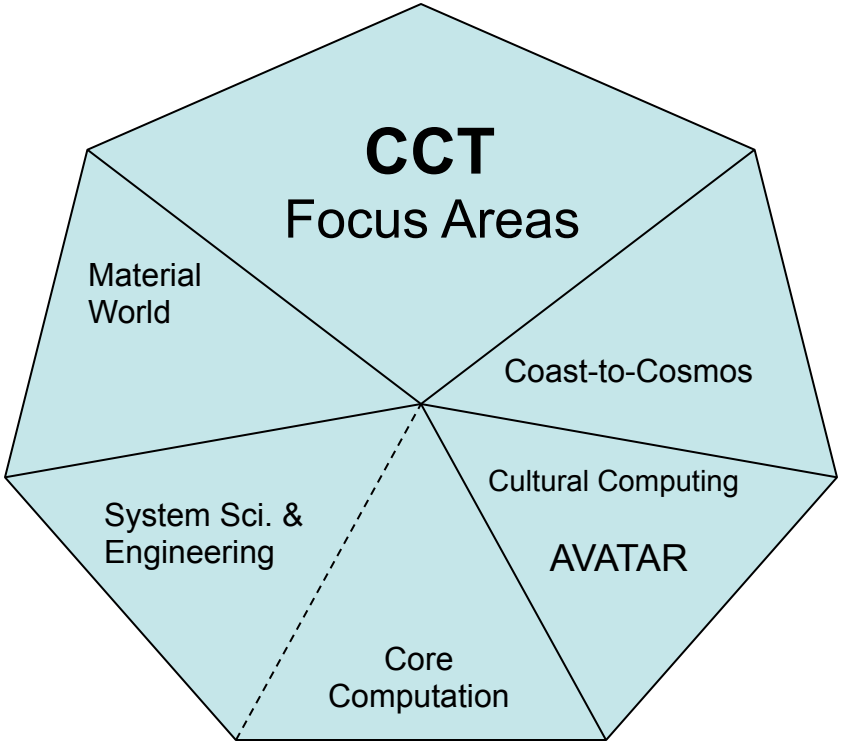
VIEW FROM WEST - PARKER COLISEUM SHOWING FUTURE PHASE BUILDING AT RIGHT

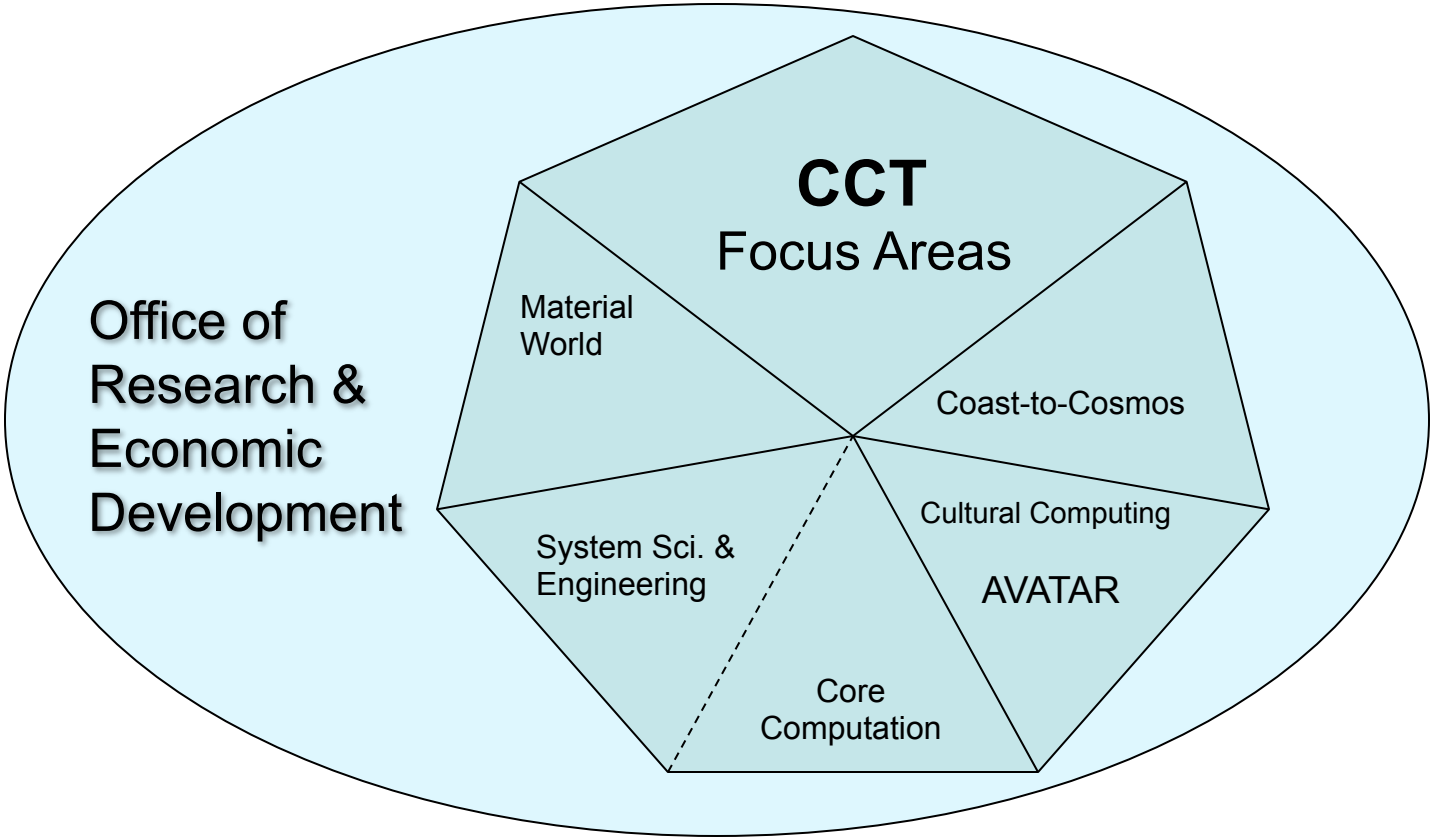
VIEW FRO

VIEW FROM WEST - PARKER COLISEUM SHOWING FUTURE PHASE BUILDING AT RIGHT

Faculty-Driven Research Activities

PART 2


CCT
Focus Areas
Material
World
Coast-to-Cosmos
Cultural Computing
AVATAR
System Sci. &
Engineering
Core
Computation


Office of Research & Economic Development
CCT
Focus Areas
Material World
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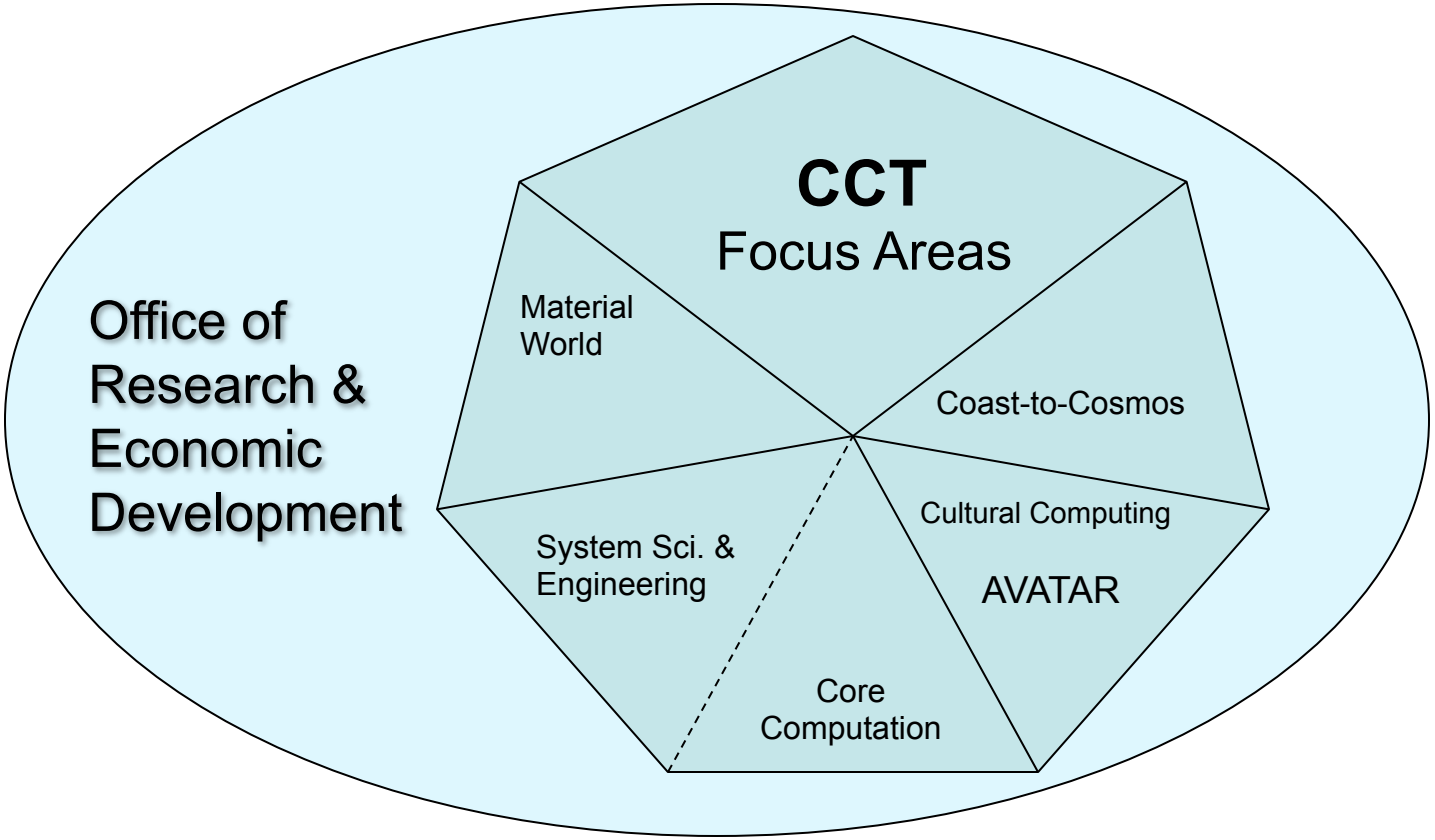
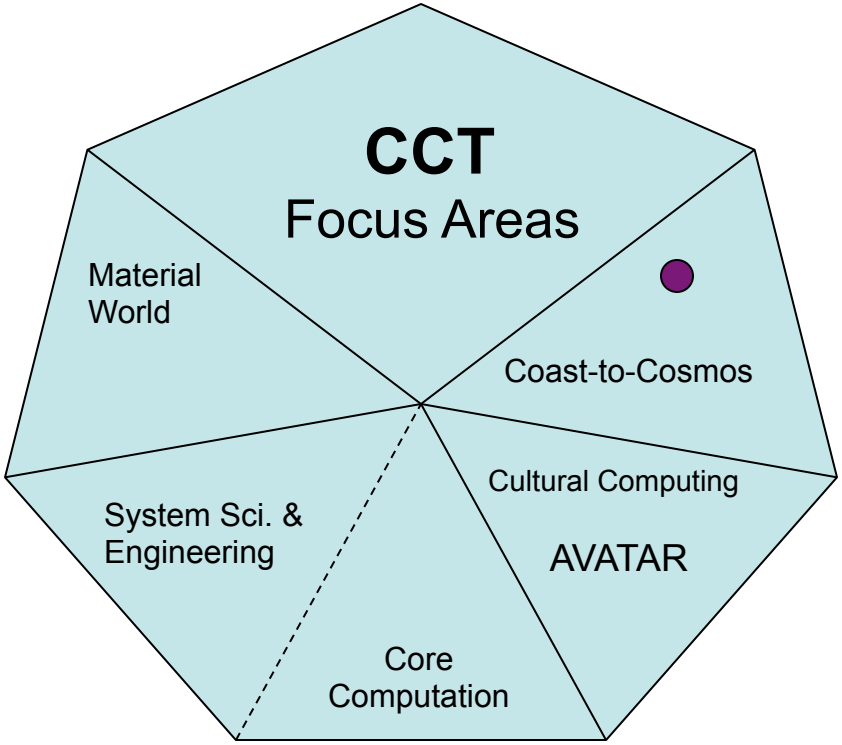


Academic Affairs Colleges

Science	***Engineering***	***Music & Dramatic Arts***	***Mass Comm***	***Business***
PHYS	Civil	----------		
MATH	PETE	***Art & Design***		
BIO	ECE			
	CS			



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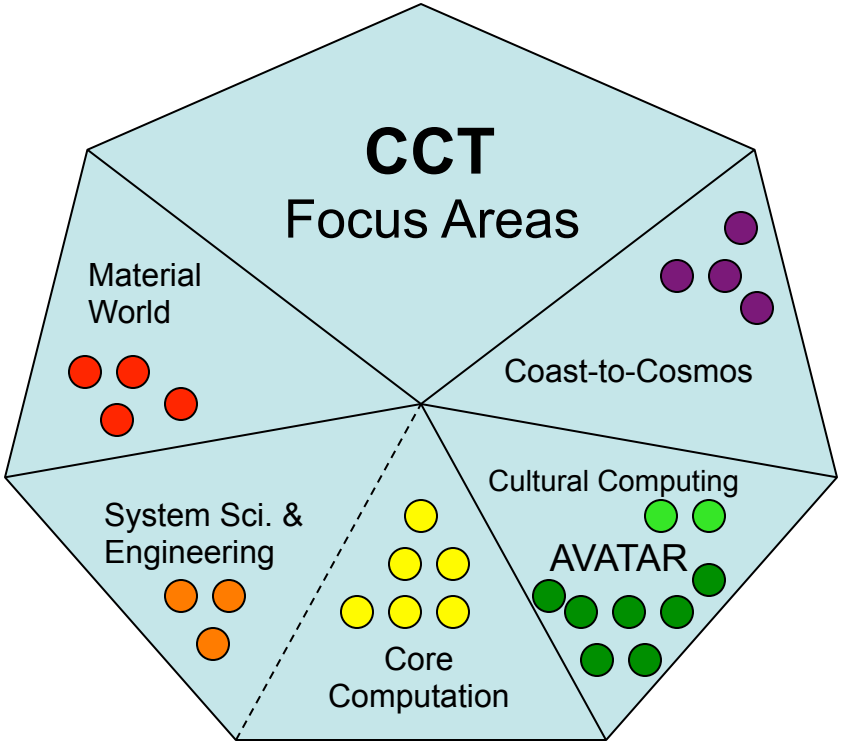
BIO	ECE			
	CS			



Academic Affairs Colleges

Science
- PHYS
- MATH
- BIO

Engineering
- Civil
- PETE
- ECE
- CS

Music & Dramatic Arts

Art & Design

Mass Comm

Business

Relevance to Biological Sciences

(*current & near term*)

- Faculty lines:
  - Michal Brylinski: 50/50 joint appointment w/ CCT; active involvement in “Material World” focus area; priority queue on SuperMike II
  - CCT has committed to help with startup funds in connection with a “computational biology / microbial metagenomics” search that is underway in Biological Science (Brylinski is on search committee)

CyberInfrastructure

PART 3

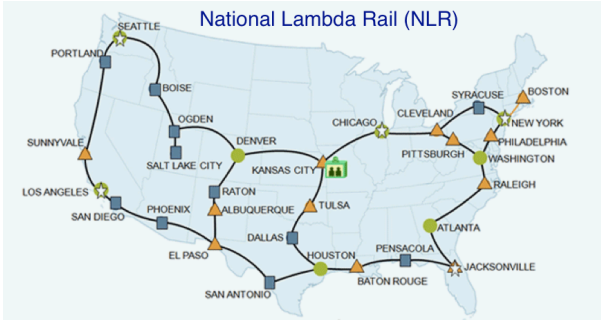
HPC in Louisiana Higher Education

LSU
CENTER FOR COMPUTATION & TECHNOLOGY

and

INFORMATION TECHNOLOGY SERVICES

(Louisiana Optical Network Initiative)



2002 : SuperMike : ~ $3M from LSU (CCT & ITS) — 11th in Top500
1024 cores; 3.7 Tflops

2006 : Tezpur : ~ $$ from LSU (CCT & ITS)
1440 cores; 15.3 Tflops

2007 : Queen Bee : ~ $5M thru BoR/LONI (Gov. Blanco) — 23rd in Top500
5440 cores; 50.7 Tflops; Became NSF-funded node on TeraGrid

2012 : SuperMike II : $2.65M from LSU (CCT & ITS)
7040 cores; 112 + 37.5 Tflops

SuperMike-II

Relevance to Biological Sciences
(*current & near term*)

- Cyber-Infrastructure:
  - Tezpur (LSU) and Queen Bee (LONI) available, free of charge to LSU researchers
  - SuperMike II recently installed at LSU
    - 440 compute nodes: at 16 cores per node ➔ 7040 cores
    - 50 nodes contain attached pair of GPUs to accelerate suitable codes
    - 8 nodes are tied together via ScaleMP ➔ even serial codes can see 2 TBytes of RAM
    - In principle, able to execute Windows OS applications
  - Network infrastructure
    - Working closely with LSU's ITS and LONI to build more steerable and higher bandwidth network connectivity across the campus and state that is smoothly integrated with national research networks
  - Data storage and management
    - Working closely with LSU's ITS and LONI to provide more adequate data storage and data management/ curation

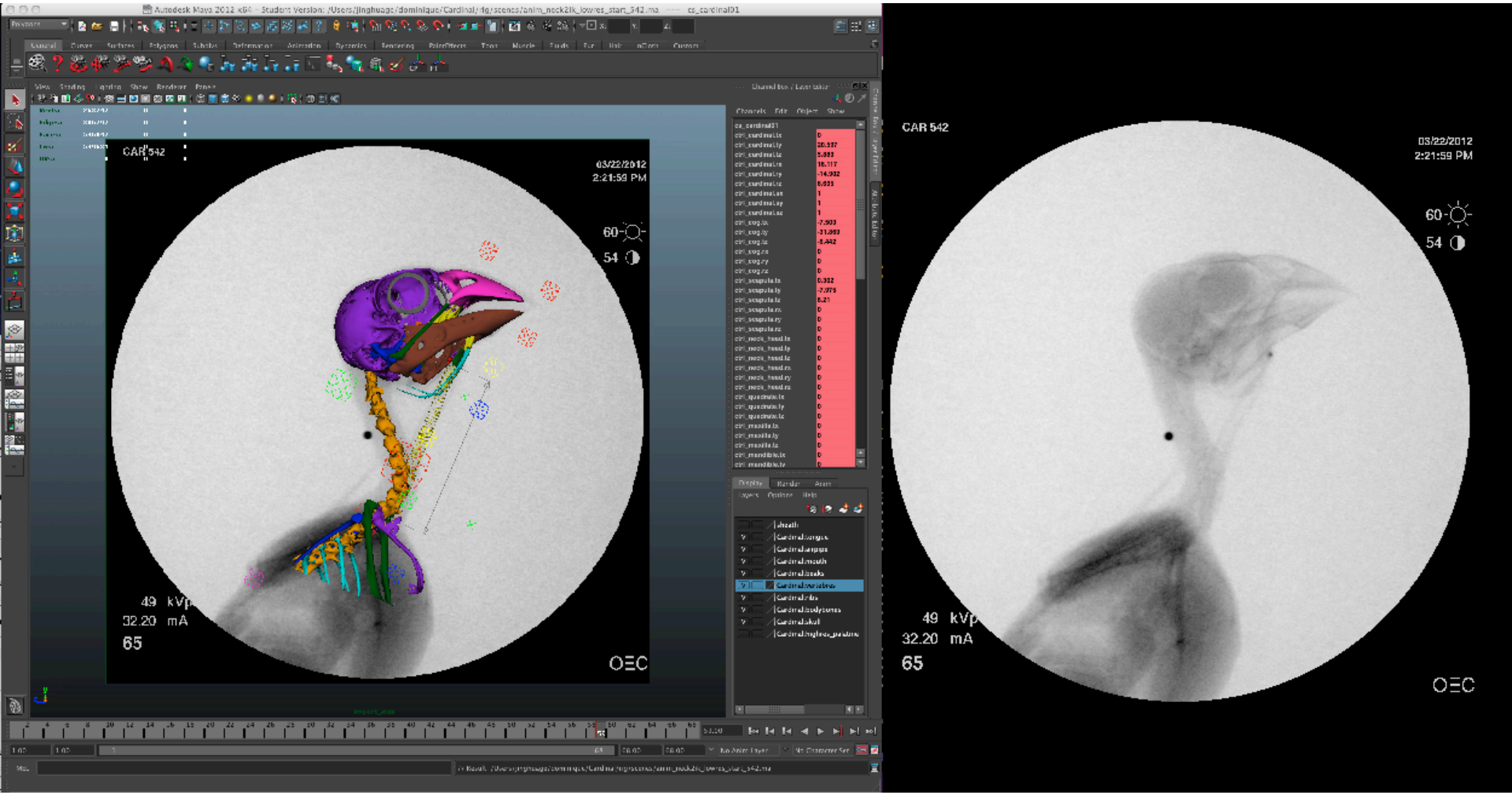
Enablement Activities

PART 4

Relevance to Biological Sciences
(*current & near term*)

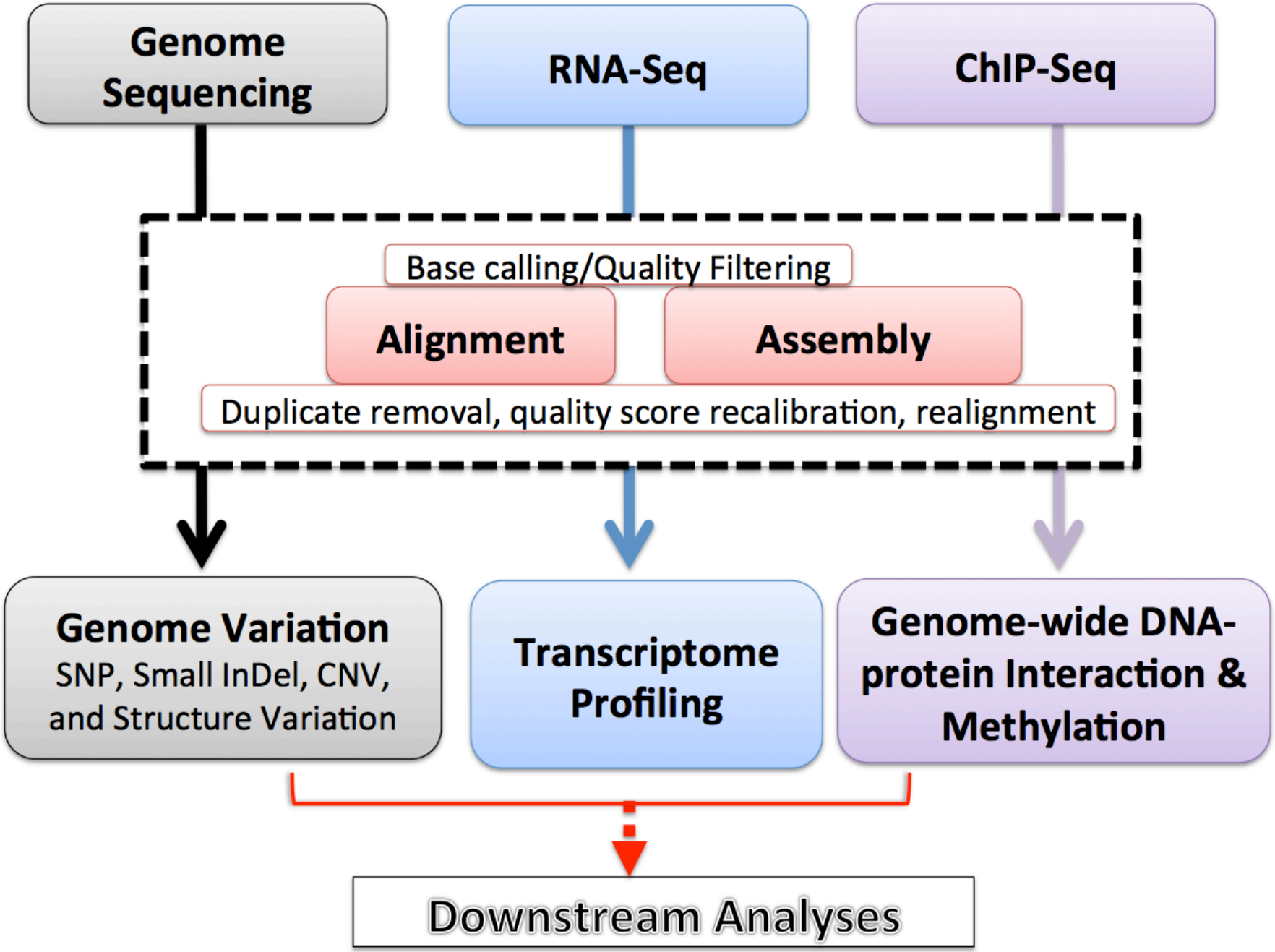
- Enablement research activities
  - Honggao Liu, CCT Deputy Director
  - James Lupo, assistant director: Takes the lead in answering any computational research questions that arise in connection with the use of LSU/LONI's high-performance computing infrastructure
  - Jinghua Ge – visualization expertise; has supported campus visualization lab and has helped develop an Honors course heavily utilizing visualization tools across the sciences. Example, interaction with Professor Homberger's research on anatomical kinematics of, e.g., birds and cats
  - Computational Biology & Bioinformatics Team: Currently 2 senior research scientists (Joohyun Kim and Nayong Kim) focused on assisting bioinformatics and broader computational biology efforts, especially in connection with LBRN = Louisiana Biomedical Research Network
  - CCT search underway to hire a "Senior Bioinformatics Computational Scientist"

Cardinal Pose



CCT Computational Biology & Bioinformatics Team

Joohyun Kim and Nayong Kim


Genome Sequencing
RNA-Seq
ChIP-Seq
Base calling/Quality Filtering
Alignment
Assembly
Duplicate removal, quality score recalibration, realignment
Genome Variation
SNP, Small InDel, CNV, and Structure Variation
Transcriptome Profiling
Genome-wide DNA-protein Interaction & Methylation
Downstream Analyses

Computational Biology/Bioinformatics Activities

Software tools

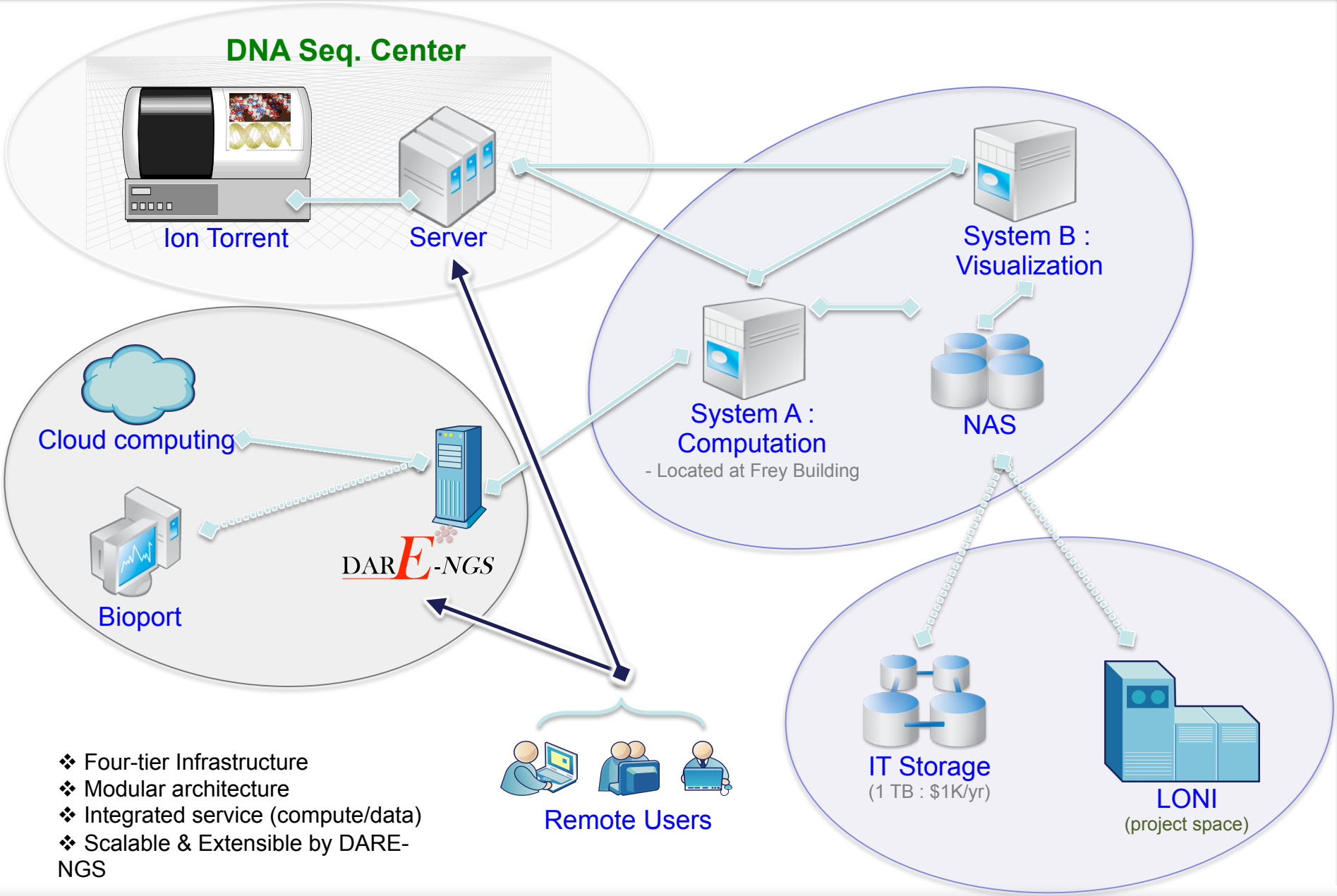
R/Bioconductor/Biopython

Protein Gene Prediction : Glimmer, GenMark.Hmm-p
ncRNA Gene Finding : Infernal, CMFinder, RNAz, Evofold
Homology Sequence Match : exonerate, BLAST
DNA motif Finding : MEME
Comparative genomics : CGView, DAVID
Functional genomics : GSEA, pathway analyses
Microarray analysis : R/Bioconductor modules
SNP : diBayes (Bioscope), BFAST, SAMTools, SOAPsnp
CNV : (Bioscope) and others
Small InDel : (Bioscope), SAMTools and others
Mapping : SSAHA2, BFAST, BWA, SHRiMP2, Novoalign, Bowtie, MAQ, Stampy, SOAP2
De Novo Assembly : EDENA, NGS Cell, ABySS, Velvet
Misc (NGS Seq. Analysis): samtools, ARTEMIS, BamView
Misc (others) : blast2GO, DAVID
RNA-Seq : TopHat/TopHat-fusion, Cufflinks, Scripture, OASES, Trinity, and othes
ChIP-Seq : MACS, and many
Phylogeny : MrBayes and others
Molecular Dynamics : NAMD, CHARMM, Gromacs, LAMMPS, TINKER
Visualization tools : VMD, IGV, BamView, Gbrowse

•Genome Analysis Framework : Bioscope, GATK

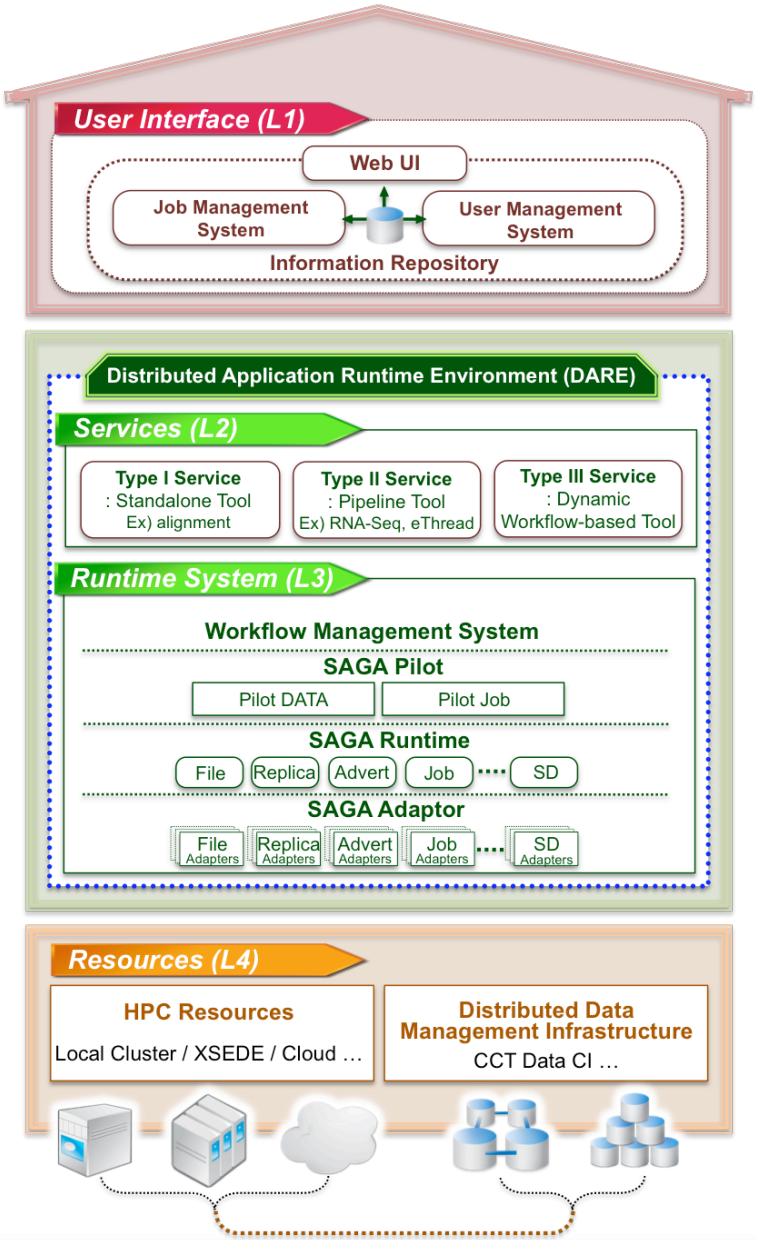
* DARE-NGS - DARE (Dynamic Application Runtime Environment)-based Science Gateway

Next-Generation Seq. Data Bioinformatics Infrastructure



- Four-tier Infrastructure
- Modular architecture
- Integrated service (compute/data)
- Scalable & Extensible by DARE-NGS

DARE Framework



DARE provides abstractions to developers of science gateways. These abstractions allow developers and scientists to focus on the unique requirements of their scientific applications and relevant workflows as opposed to focus on the "plumbing" of how to submit ensembles of simulations to several supercomputers concurrently and archive their results. DARE is the natural evolution of science gateway middleware. As resource platforms, network capabilities and data repositories grow in size, number and vary in interface, the emergence of a unifying framework was inevitable. Many of the critical features of the DARE framework are provided by SAGA and the Pilot-Job capability: SAGA-BigJob SAGA demonstrated the capability (and usefulness) of overcoming utilization issues associated with distributed compute and data resources, complex multi-level workflows and run-time decision making. Building a science gateway framework on top of SAGA was the next logical step. The DARE framework's distinguishing features include support for HPDC infrastructure and application/application workflow agnosticism.

DARE Framework

Available Services – three different types

Service Type	Type I	Type II	Type III
Service Description	Standalone Single Tool	Pipeline Tool	Dynamic Workflow-based Tool
Example Target Application	Mapping	ChIP-Seq, RNA-Seq	ChIP-Seq, RNA-Seq
Example of Existing Tools	Bfast, BWA, Bowtie, ABySS	Mapping+MACS, TopHat-Fusion, Trans-ABySS, Hydra, GATK	N/A

Upcoming Services

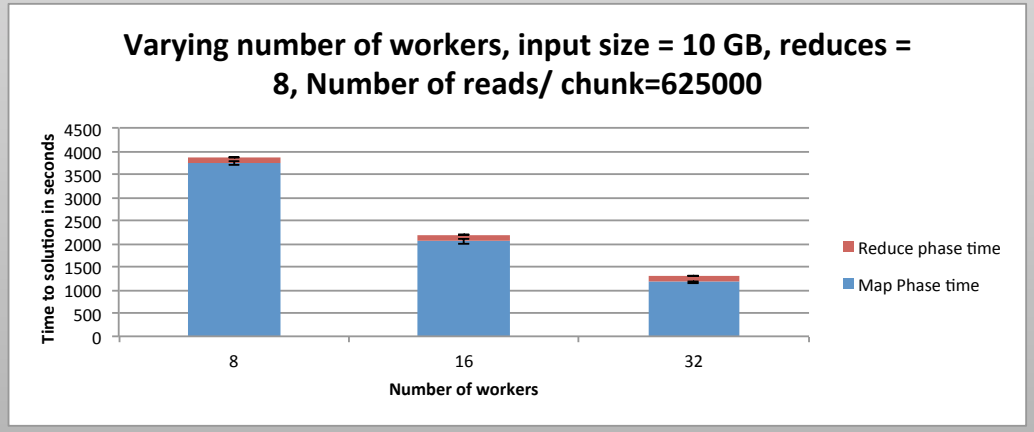
RNA-Seq pipelines
Structural Bioinformatics : eThread

DARE-NGS

Scale out performance for DNA sequence mapping using BFAST on HPC

Compute System	# of cores	# of tasks	Task Concurrency	Bfast (mapping)
Workstation	4	8	No	≈18 h (or 72 h)
Ranger (HPC)	64	4	Yes	6.5 h
Ranger (HPC)	128	8	Yes	3.4 h
Ranger (HPC)	256	16	Yes	1.95 h

Scale out performance for DNA sequence mapping using BWA with Map-Reduce



Relevance to Biological Sciences

(*current & near term*)

- Enablement research activities
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Visiting Panelists
(February 2012)

Boore, Jeffrey
CEO, Genome Project Solutions, Inc.
Adjunct Professor, Department of Integrative Biology, UC-Berkeley
http://genomeprojectsolutions.com/Personal_home_pages/Jeffrey_Boore.html

Cherbas, Peter
Director, Center for Genomics and Bioinformatics
Professor, Department of Biology, Indiana University
http://www.bio.indiana.edu/faculty/directory/profile.php?person=cherbas

Collins, Jack
Director, Advanced Biomedical Computing Center
National Cancer Institute, Frederick, Maryland
http://isp.ncifcrf.gov/abcc/abcc-staff/abcc-staff-bio/?id=12

Jongeneel, Victor
Director of Bioinformatics
Institute for Genomic Biology, University of Illinois
http://www.ncsa.illinois.edu/News/10/0301Jongeneeljoins.html

*Kissinger, Jessica
Director, Institute of Bioinformatics
Associate Professor, Department of Genetics, University of Georgia
http://www.genetics.uga.edu/people_bio_kissinger.html

Pfrender, Michael
Associate Professor, Department of Biological Sciences
Evolutionary & Ecological Genomics Lab, University of Notre Dame
http://biology.nd.edu/people/faculty/pfrender/

Quackenbush, John
Professor, Department of Biostatistics, Harvard School of Public Health
http://134.174.190.199/faculty/john-quackenbush/

Thomas, W. Kelley
Director, Hubbard Center for Genome Studies, University of New Hampshire
http://www.unh.edu/news/cj_nr/2011/feb/bp03genome.cfm

Wang, Yue (Joseph)
Director, Computational Bioinformatics and Bio-imaging Laboratory
Bradley Department of Electrical & Computer Engineering, Virginia Tech
http://www.ece.vt.edu/faculty/ywang.php

Strengthening Bioinformatics Research at PBRC and LSU

Expert Panel Recommendations

15-17 February 2012

2. Recruit and hire a senior scientist with experience in coordinating biologists and bioinformatics in a research center environment
    a. This hire should be placed in the CCT and charged with coordinating the more centralized bioinformatics model described in recommendation #1, especially to support the analysis of genome sequences
    b. This should be a joint appointment across Biological Sciences, CCT and PBRC
    c. This hire should coordinate the research and service activities of "professional" hires identified in recommendation #3b
    d. In stages, this hire should also develop and coordinate an outreach component across the state and outside the university system – see related recommendation #6

Strengthening Bioinformatics Research at PBRC and LSU
Expert Panel Recommendations

15-17 February 2012

3. Hire a mix of researchers whose collective expertise spans a variety of areas of emphasis
    a. Make a few key tenure-track faculty hires that are "genome enabled" in order to increase usage of the genomics and bioinformatics cores and increase interactions between biologists and research scientists with computational expertise
    b. Develop "professional" positions that are not tenure-track but that are intended to be strongly collaborative and service oriented
        i. These positions should probably largely reside within the CCT
        ii. Service efforts should be coordinated by the senior scientist described in recommendation #2
        iii. To offset cost of additional staff positions, recognize the involvement of the CCT on grant proposals and direct additional F&A to the CCT when these are successful applications
    c. Consider making "research faculty" hires as well
    d. Lay out a thoughtful strategy regarding where new positions will reside and how appropriate joint appointments might stimulate interdisciplinary collaborations

Bioinformatics Hire Search Committee

- Brown, Jeremy (Biological Sciences)
- Canavier, Carmen (LSUHSC Biology & Anatomy)
- Kim, Joo (Biological Sciences)
- Macaluso, Kevin (SVM's Pathobiological Sciences)
- Monroe, Todd (Biological & Agricultural Engineering) – committee chair
- Mores, Chris (SVM's Pathobiological Sciences)
- Salbaum, Michael (Pennington Biomedical Research Center)
- Ullmer, Brygg (CCT and Computer Science)

Senior Bioinformatics Computational Scientist

(draft advertisement)

- The Center for Computation & Technology (CCT) at Louisiana State University invites applications for a senior research scientist position in Computational Bioinformatics, broadly defined. The successful candidate will recruit and lead an Interdisciplinary Research Support Group (IRSG) that will support and integrate data-intensive and computationally demanding research activities across various academic units on LSU's main campus, at the LSU School of Veterinary Medicine, the Pennington Biomedical Research Center, and LSU's Health Sciences Centers. The IRSG will support research in genomics, bioinformatics, biostatistics, biomolecular structure/function, systems biology modeling, computational neuroscience, and other areas.

- The new leader of the IRSG will be charged with mobilizing this infrastructure to support the cutting-edge, interdisciplinary research activities described above. S/he will participate in and lead the development of extramural grant proposals. Equally important, s/he will develop programs to assist faculty and scientists in their use of bioinformatics and computational resources -- by individual mentoring and by workshops and tutorials. The IRSG leader will be encouraged to develop collaborative ties with industrial scientists across Louisiana.

- Required Qualifications: Ph.D. in biology, computational science, or a related area with emphasis on bioinformatics data analysis; five years of experience.

- Additional Qualifications Desired: Experience leading bioinformatics and biostatistics projects, teams and software use and development. Experience with common software development languages and tools, software design, and architecture and with the scripting tools commonly used by bioinformaticists: PERL, GALAXY, R/ Bioconductor, etc. Experience with large dataset management specific to next-generation sequencing. Experience in the development of web interfaces to bioinformatics tools. Experience with high-performance computing, parallel programming and/or programming frameworks. Experience using virtual collaborative environments.

- Appointment and salary will be commensurate with experience and qualifications. This is a non-tenure track research position.

THANK YOU