



LA-SIGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Project Overview

Mark Jarrell

LSU, Physics and Center for Computation
and Technology

SCIENCE DRIVER 1

Correlated Materials

SCIENCE DRIVER 2

Energy Materials

SCIENCE DRIVER 3

Superconducting
Materials



THE UNIVERSITY of
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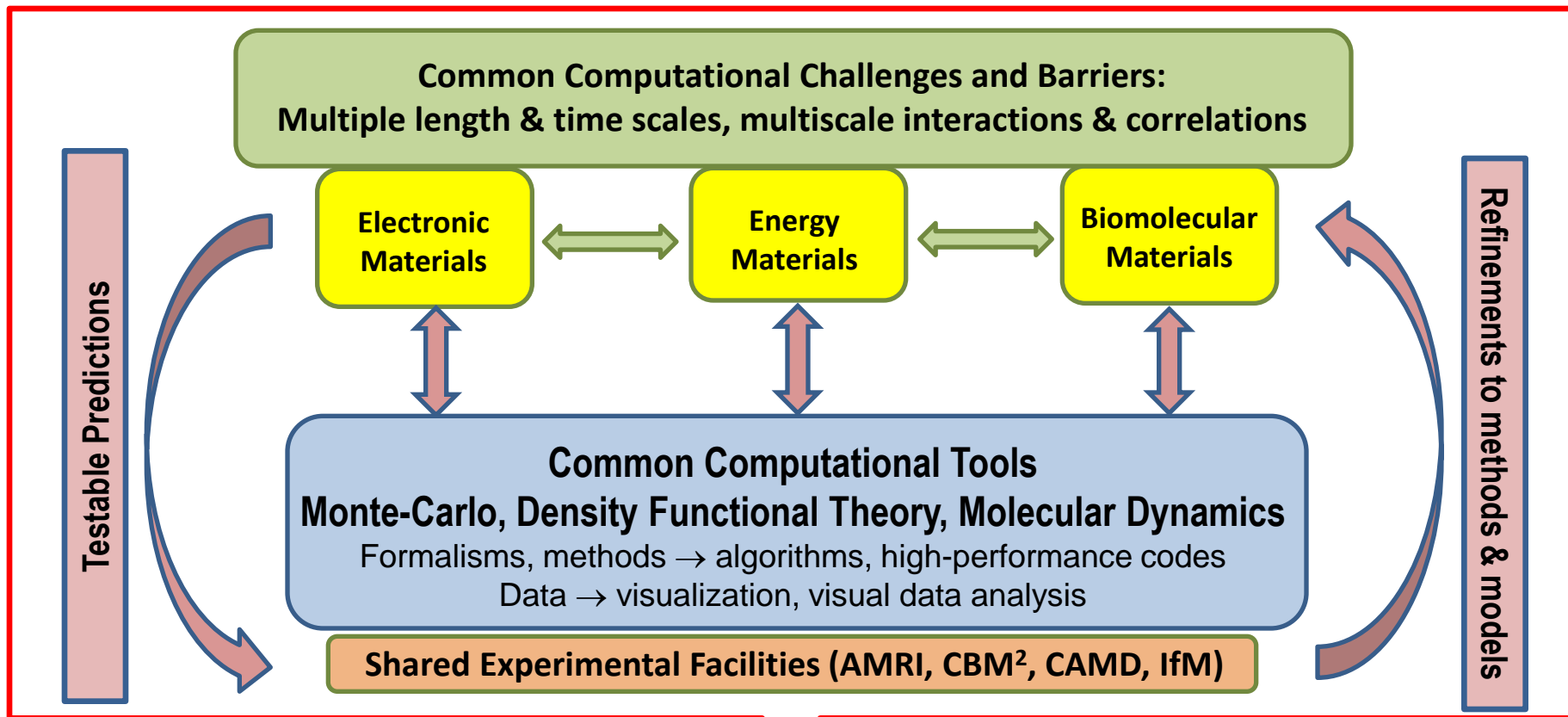


LA-SiGMA in a Nutshell



- The largest grant awarded by NSF to the State of Louisiana.
- **Research:** Develop computational methods and tools capable of anticipating the properties of materials just like pharmaceutical companies are able to use computational modeling to narrow down potential candidates for various drugs.
- **Education & Workforce Development:** Increase the numbers of students who choose to major in science, technology, engineering and mathematics (STEM) in college, get engaged in research, and pursue advanced degrees. Specialized short courses for 2-year college students and teachers.
- **Diversity:** A special emphasis is placed on recruiting women and under-represented minorities into STEM disciplines and helping them succeed – faculty, postdocs and students.
- **External Engagement:** RET programs, LPB, and science museums.
- **Sustainability:** Build strong inter-institutional research teams that become competitive for large scale national awards; position the State to win a major federally funded center of excellence.

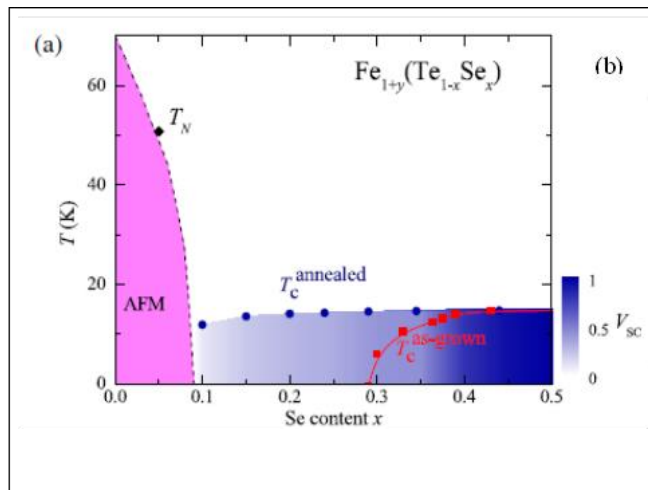
LA-SiGMA Research Roadmap



OUTCOMES

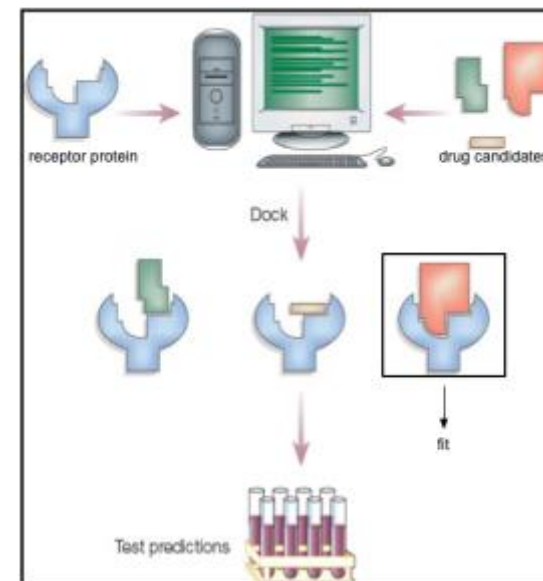
Strong Multidisciplinary and Multi-Institutional Research Teams
Multiscale Simulation Tools for 21st Century Computing Environments
Statewide Research and Education Programs in Materials Science
National Center of Excellence in Simulation-Guided Materials Applications

Common Problems, Common Tools

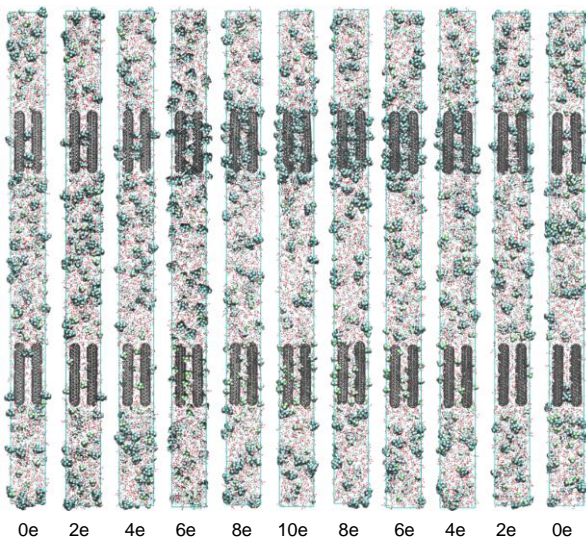


Some projects
you will hear
about today

SD1: Electronic and Magnetic Materials
Competing phases and criticality



SD3: Biomolecular Materials. Drug
discovery by docking



SD2: Energy Materials. First simulation
of filling of CNT forest

- Many length and time scales
- Complex and competing phenomena
- Common tools
 - Monte Carlo
 - Molecular Dynamics
 - Density Functional Theory



Science Drivers

**Electronic
Materials**

Magnetic materials,
Superconductors

Leaders:
Jarrell (LSU),
Perdew (Tulane)

**Biomolecular
Materials**

Biopolymers,
Drug Delivery
vehicles

Leaders:
Ashbaugh (Tulane),
Moldovan (LSU)

**Common computational
tools bind the three
science drivers together.**

**Monte-Carlo,
Density Functional
Theory,
Molecular
Dynamics**

**Energy
Materials**

Electrical energy storage
materials (capacitors,
batteries), Catalysts

Leaders:
Pratt (Tulane),
Wick (LA Tech)

**CyberInfrastructure makes
research and collaboration
possible:**

- LONI
- HD Polycom
- Next Gen computing platforms

Leverage

2012/3: SuperMike + SuperMIC

2010: LA-SiGMA (EPSCoR RII)

2007: CyberTools (EPSCoR RII)

2007: LONI Institute

~2007

The "Queen Bee"

Dell HPC Clusters

~2005

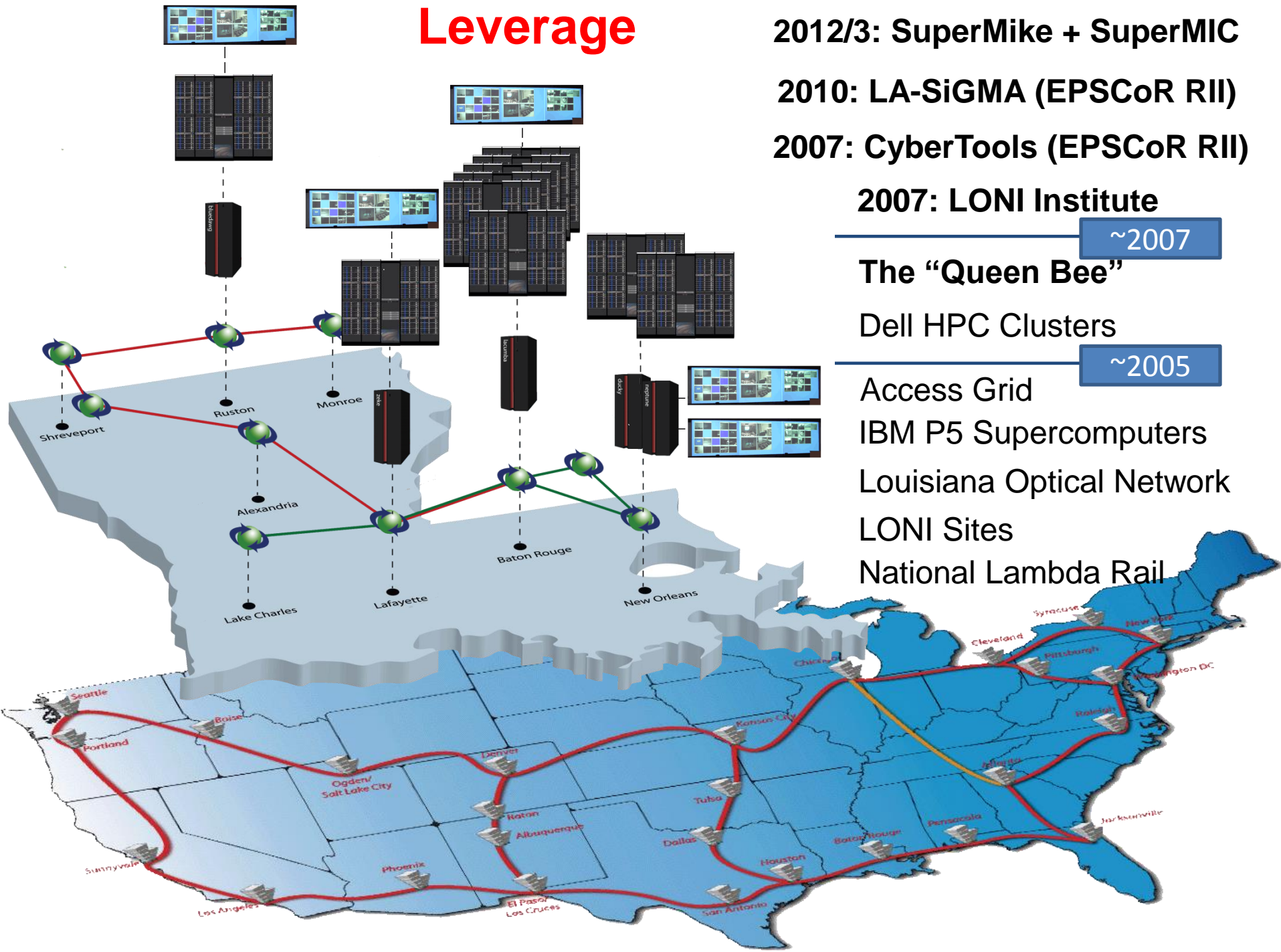
Access Grid

IBM P5 Supercomputers

Louisiana Optical Network

LONI Sites

National Lambda Rail



Significant Changes in the last year



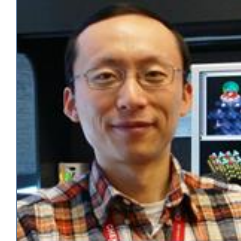
1. Dropped H-storage from Science Driver 2 *
 - a. Added Li-ion batteries and electrochemical sensors
2. Increased Emphasis on Data Management
 - a. Data Semantics Workshop summer 2013.
 - b. Partnership with TACC (Corral)
 - c. Data exchange
 - d. Projects incorporating metadata
3. Increased Collaboration with EFRC
 - a. Science Driver 2 presentation
4. Very large number of new hires
 - a. 10 new hires!
 - b. Large increase in SD2 Energy Research

*This change was made in response to the ERB comments in 2012 and is reflected in the revised Strategic Plan accepted by the NSF.

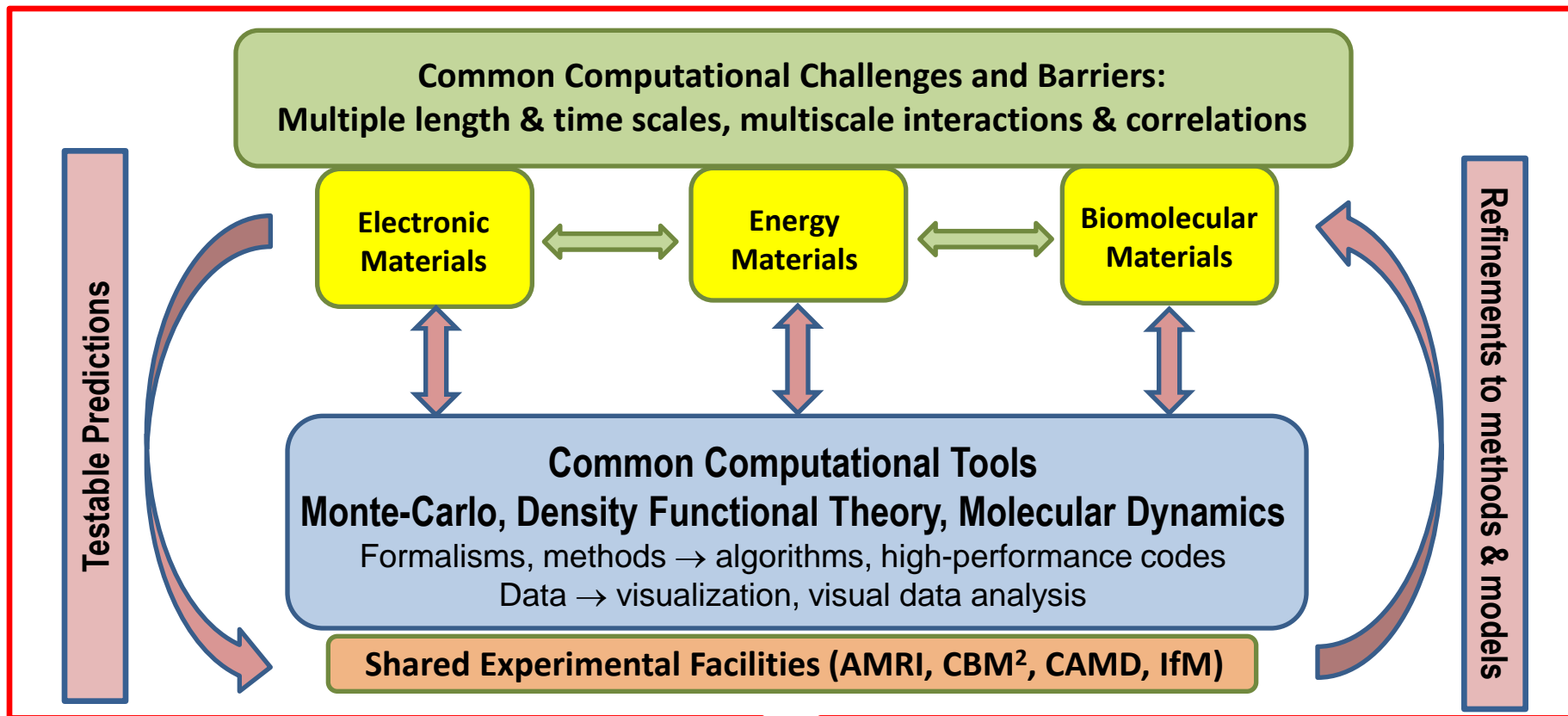
LA-SIGMA Recent Hires



- Anne Robinson – Chair of Chemical & Biomolecular Department, Catherine and Henry Boh Professor of Engineering, Tulane.
- Bill Shelton – Computational Physics and Chemistry, expert in HPC and Big Data, LSU.
- Kevin Riley – First Computational Chemist, Xavier.
- Michal Brylinski – Recognized Among Nation’s Top Junior Faculty, Computational Biology, LSU.
- Revati Kumar – Computational Chemistry, LSU.
- Doug Chrisey – Cornelia and Arthur Jung Chair in Materials Engineering, Tulane.
- Ken Lopata – Computational Chemistry, LSU.
- Ye Xu – Computational Chemistry, LSU.
- Prabhu U Arumugam – Carbon Nanochemistry, LA Tech
- Clint Whaley – ScaLAPACK, ATLAS, Computer Science, LSU
- Dhruva Chakravory, Computational BioChemistry, UNO



LA-SiGMA Research Roadmap



OUTCOMES

- Strong Multidisciplinary and Multi-Institutional Research Teams ✓
- Multiscale Simulation Tools for 21st Century Computing Environments ✓
- Statewide Research and Education Programs in Materials Science ✓
- National Center of Excellence in Simulation-Guided Materials Applications

Remaining Symposium Agenda for Today

(10 minutes or break for Q&A after each talk)



1. Science Drivers and Computation

- a. 9:10-9:30, SD1: Electronic and Magnetic Materials
- b. 9:30-10:00, Break**
- c. 10:00-10:20, SD2: Materials for Energy Storage and Generation
- d. 10:30-10:50, SD3: Biomolecular Materials
- e. 11:00-11:20, Computational Tools for Multiscale Simulations
- f. 11:30-11:45, Data Management Plan
- g. 11:45-2:00, Lunch and poster presentation**

2. Assessment and Broader Impacts

- a. 2:00-2:15, Diversity and Workforce Development
- b. 2:25-2:40, External Engagement, Sustainability
- c. 2:50 – 3:20, Recipients of EPSCoR awards, and Q&A
- d. 3:20 – 3:35, Graduate Student Retreat
- e. 3:35 – 3:50, Evaluation and Assessment (Dunn)
- f. 3:50 – 4:05, Break**

3. Planning Session

- a. 4:05 – 5:15, ERB and DAC deliberations
- b. 5:30, Concluding Remarks (Khonsari)



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Questions?



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