LA-Sigma Share-a-Thon

Chris Campbell

David Andersen

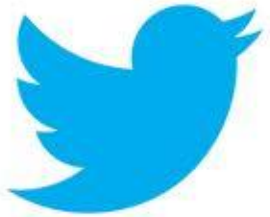
Brad Burkman

Karen Higuera

Chris Hynes

Mary Beth McCoy

But feel free to (silently)….



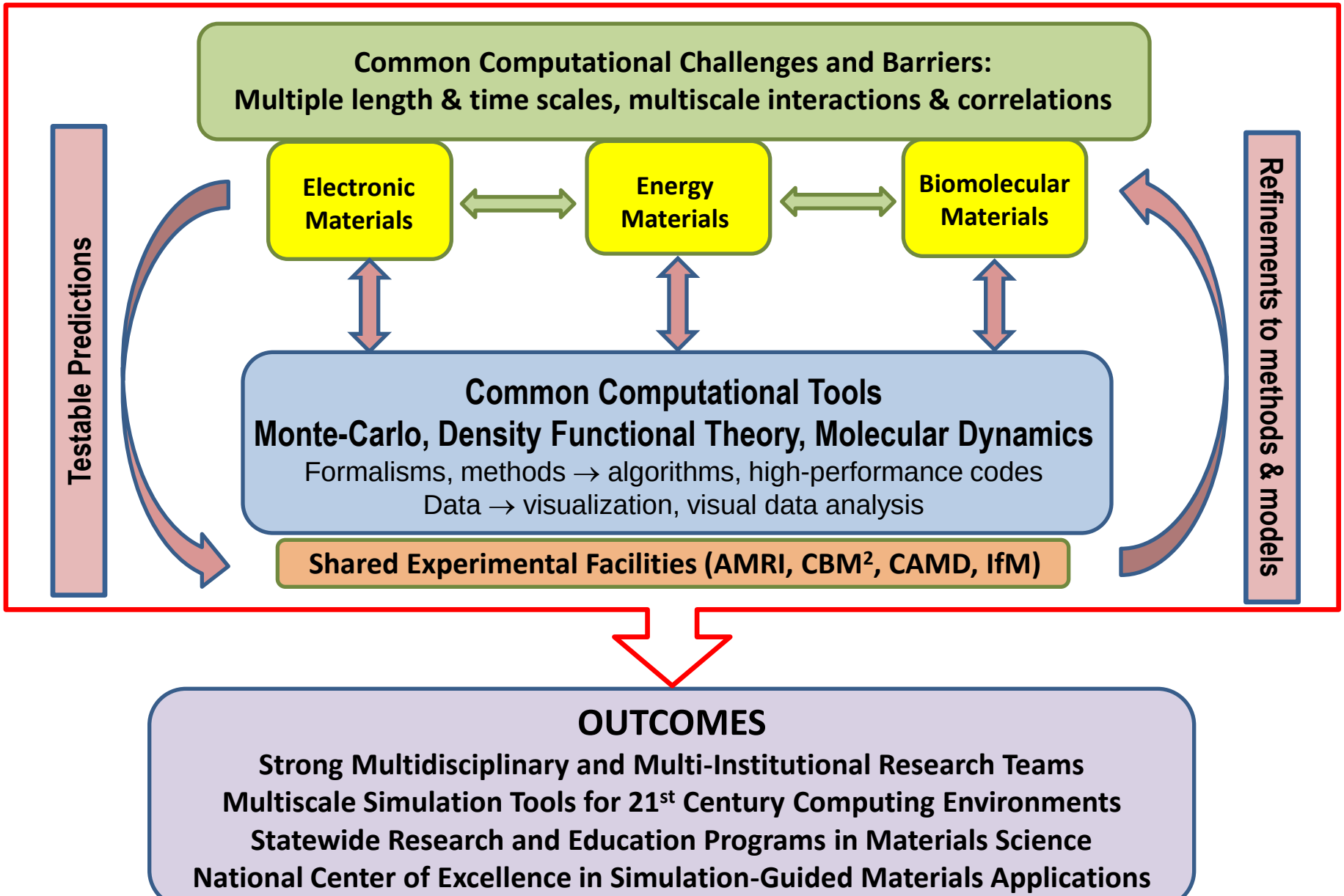
Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA)

- Seven campuses
- Five research universities
- Two predominantly undergrad institutions
- Three HBCU's
- 55 senior investigators
- Additional ~10 collaborators (in-state and out)
- ~60 graduate students and postdocs

PI: Michael Khonsari, EPSCoR Director
Assoc. Commissioner for Sponsored Programs

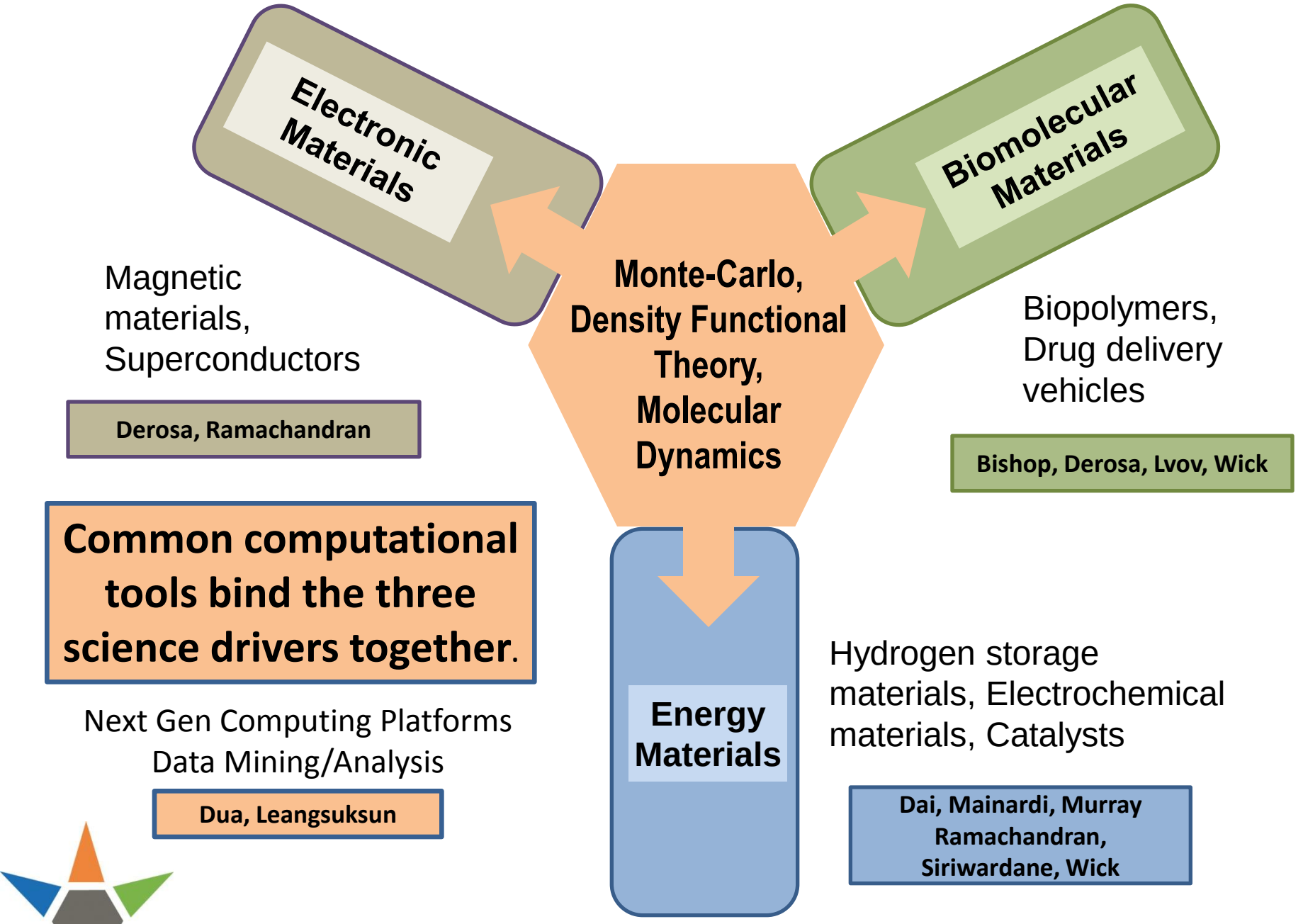
Co-PI's:
Mark Jarrell, LSU
Randy Hall, LSU
Lawrence Pratt, Tulane
B. Ramu Ramachandran, LA Tech

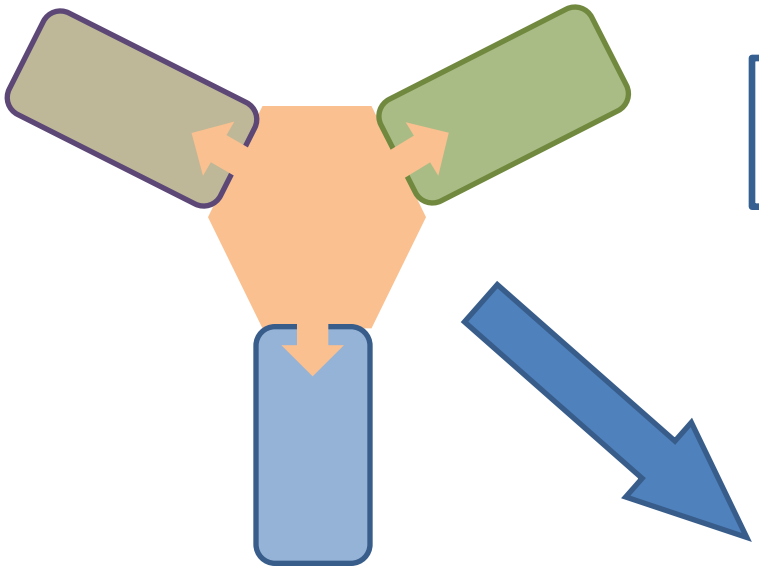
LA-SiGMA Research Roadmap



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


Electronic Materials
Biomolecular Materials
Monte-Carlo, Density Functional Theory, Molecular Dynamics
Energy Materials
Magnetic materials, Superconductors
Derosa, Ramachandran
Biopolymers, Drug delivery vehicles
Bishop, Derosa, Lvov, Wick
Common computational tools bind the three science drivers together.
Next Gen Computing Platforms
Data Mining/Analysis
Dua, Leangsuksun
Hydrogen storage materials, Electrochemical materials, Catalysts
Dai, Mainardi, Murray
Ramachandran, Siriwardane, Wick



Our Logo

LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

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.

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What is LONI?

Louisiana Optical Network Initiative

Vision and Leadership from Ed Seidel, Gov. Blanco, and Louisiana Board of Regents

High-bandwidth optical network linking graduate-degree granting institutions in the state.

HPC hardware at 6 institutions

LONI layers

2010: LA-SiGMA (EPSCoR RII)

2007: CyberTools (EPSCoR RII)

2007: LONI Institute

~2007

The "Queen Bee"

Dell HPC Clusters

~2005

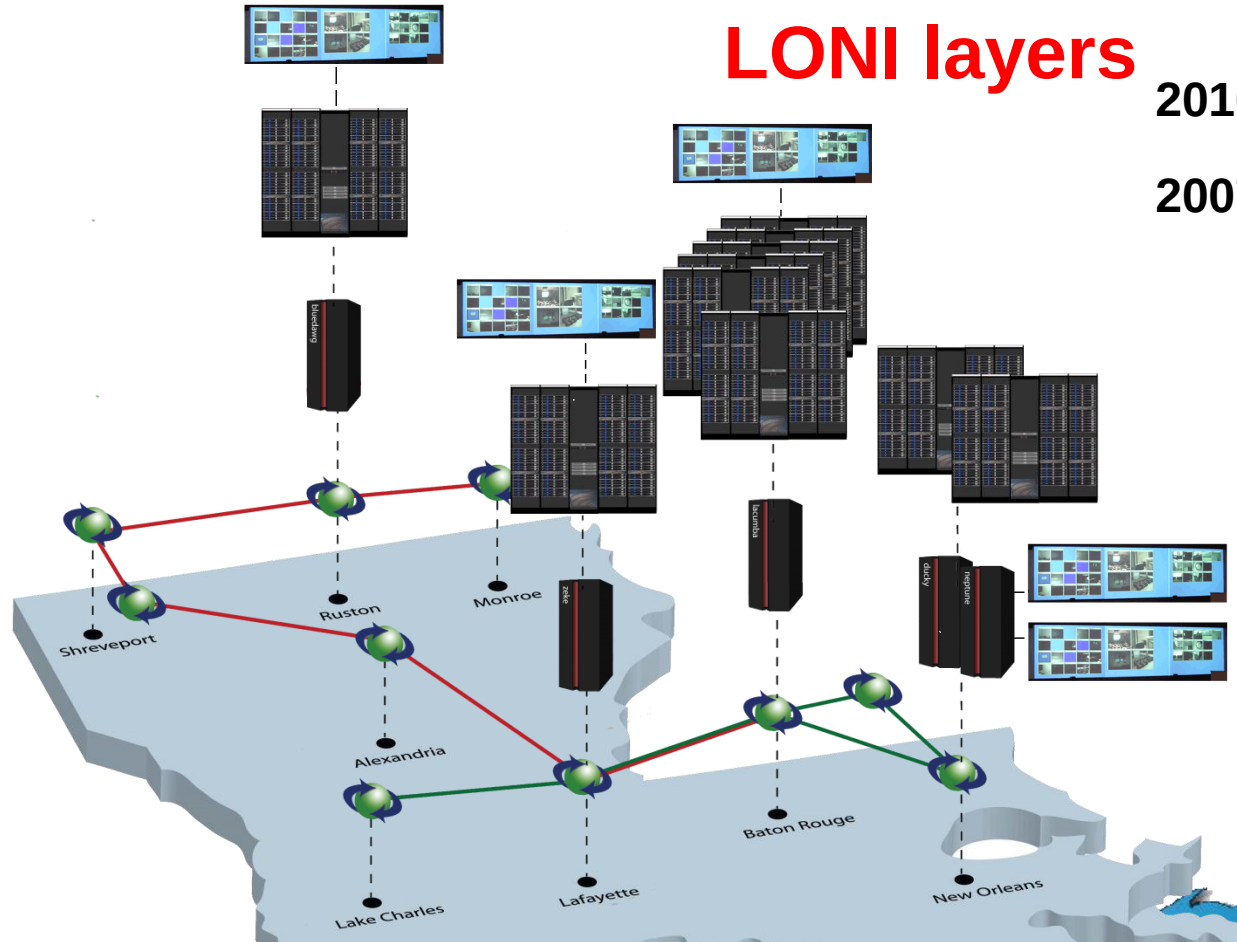
Access Grid

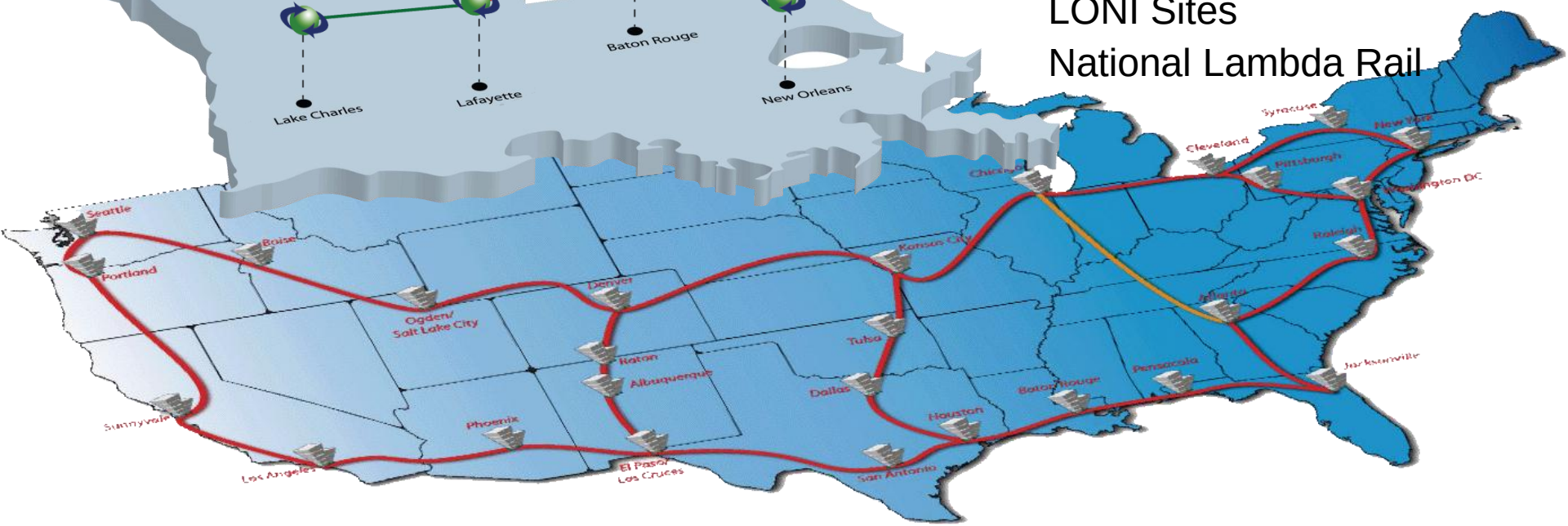
IBM P5 Supercomputers

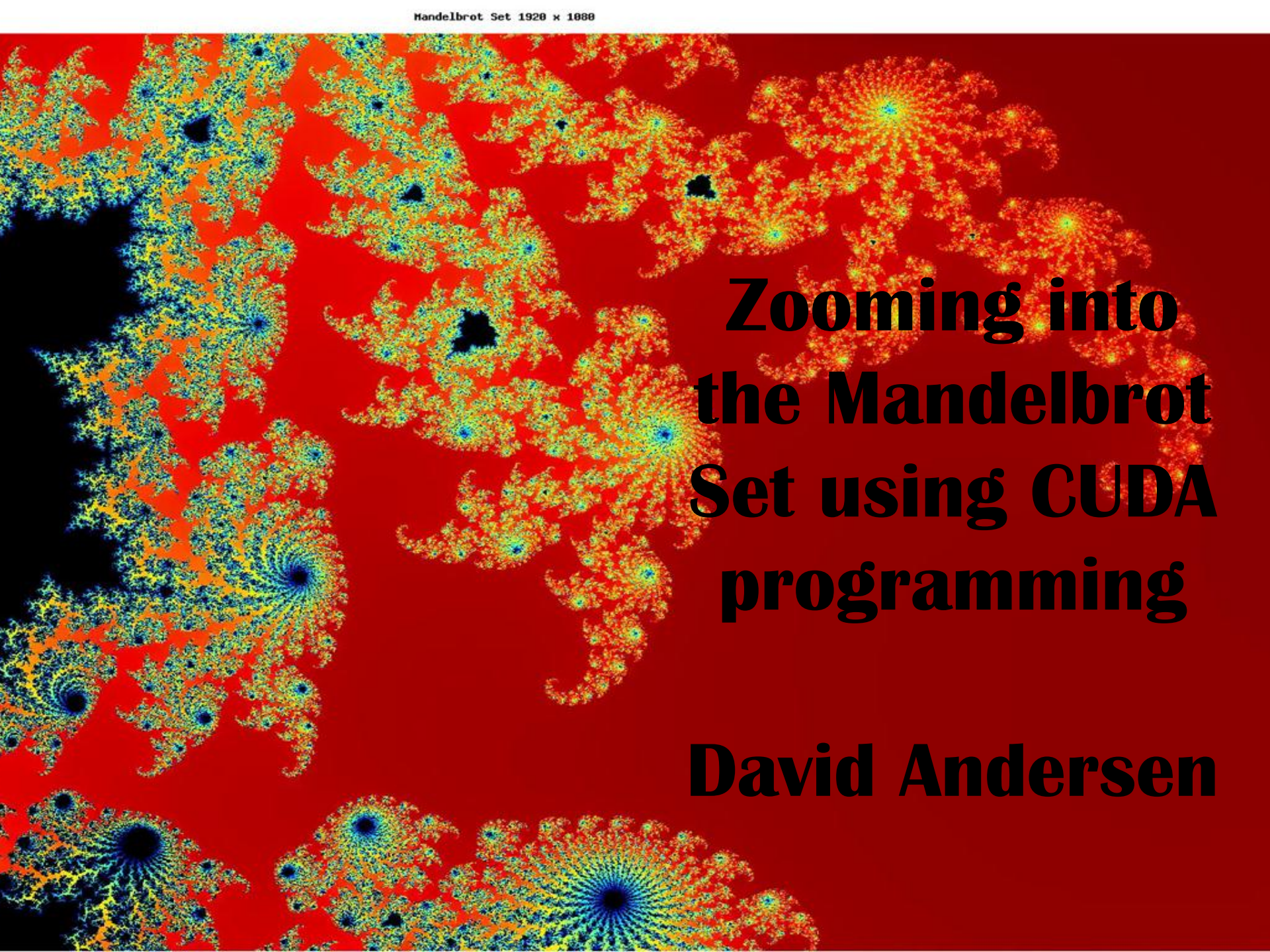
Louisiana Optical Network

LONI Sites

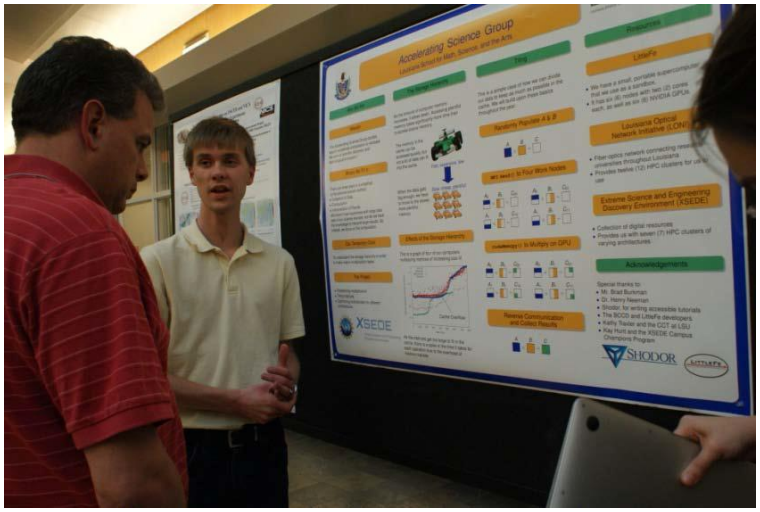
National Lambda Rail






Mandelbrot Set 1920 x 1080
Zooming into the Mandelbrot Set using CUDA programming
David Andersen

“Accelerating Science” Student HPC Research Group
Brad Burkman, Louisiana School



LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

LittleFe
Computational Science Education on the Move
http://LittleFe.net/

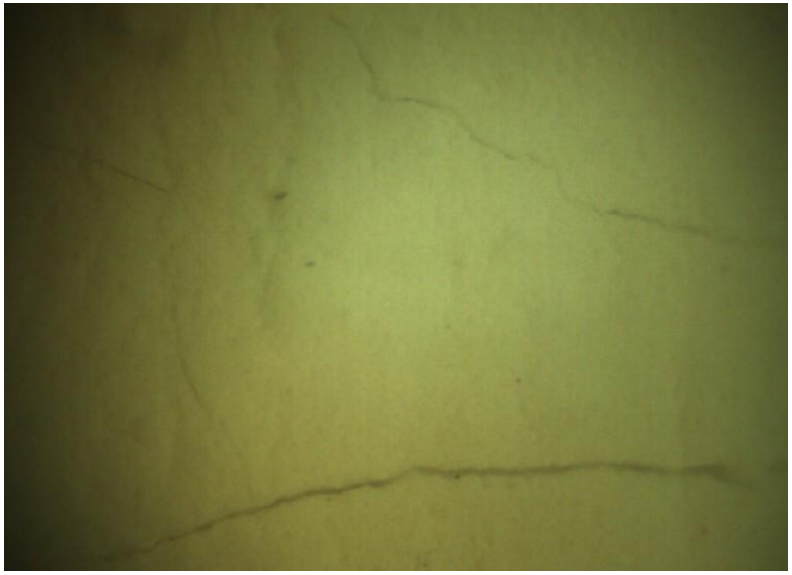
XSEDE
Extreme Science and Engineering Discovery Environment

LSU Center for Computation & Technology

OU Supercomputing Center for Education & Research
OSCER
University of Oklahoma

SHODOR

NOx Sensors in the Exhaust Systems of Automobiles



Yttria substituted zirconia sample

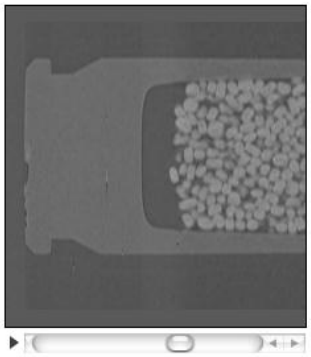
Scandia substituted zirconia sample

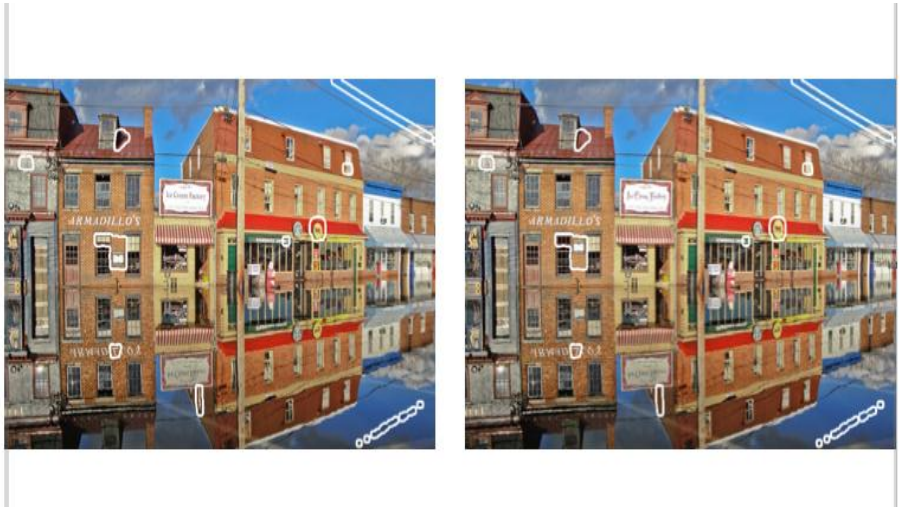
Karen Higuera
Dr. Erica Murray

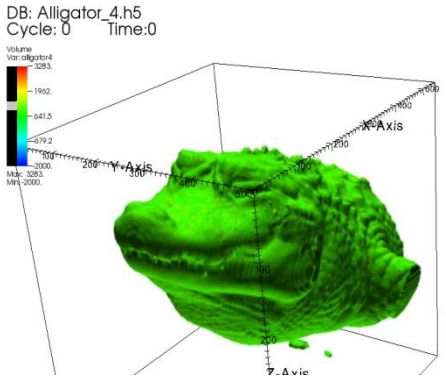
LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

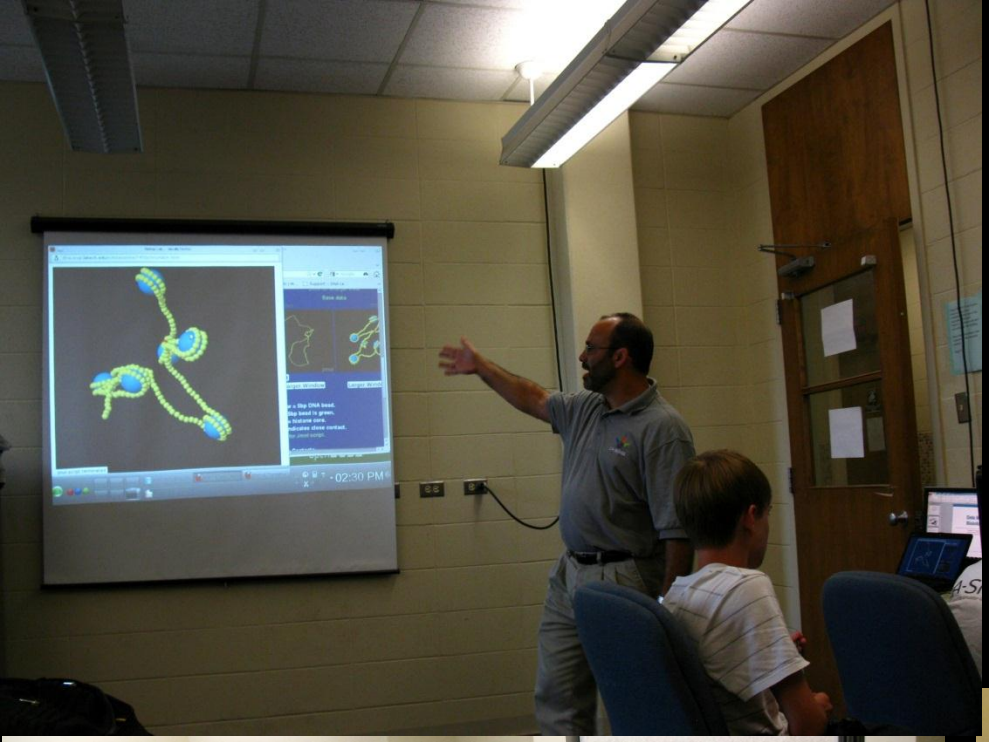
Implementing the LA-SiGMA Experience: Data set visualization – merging of art, math, and science

Christopher J. Hynes
Louisiana School for Math, Science and the Arts









Mary Beth McCoy
Ouachita Jr. High

Modeling DNA

Dr. Tom Bishop