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# EPSCoR Symposium 2012

LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

# Louisiana's Research Infrastructure Improvement Strategy 2010-2015

## Project Overview

**Michael Khonsari**

Louisiana EPSCoR Project Director

Associate Commissioner for Sponsored Programs Research & Development, Louisiana Board of Regents

Professor and Dow Chemical Endowed Chair in Rotating Machinery, LSU College of Engineering

# External Review Board

**James Hoehn**
*EPSCoR/IDeA*

**Dr. Vincent McKoy**
*Caltech*

**Dr. William Lester**
*UC Berkeley*

**Dr. Harold Silverman**
*SUNY (retired)*

**Dr. Valerie Taylor**
*Texas A&M*

**Dr. Susan Sinnott**
*University of Florida*

# Diversity Advisory Council

**Shelia Edwards Lange**
*U Washington*

**Jenna Carpenter**
*Louisiana Tech*

**William Lester**
*UC Berkeley*

**Betsy Willis**
*Southern Methodist U*

**Isiah Warner**
*LSU*

**Stephanie Adams**
*Virginia Commonwealth U*

**DiOnetta Jones**
*MIT*

**Juana Moreno**
*LSU*

# Integral Collaborations

*Louisiana EPSCoR*

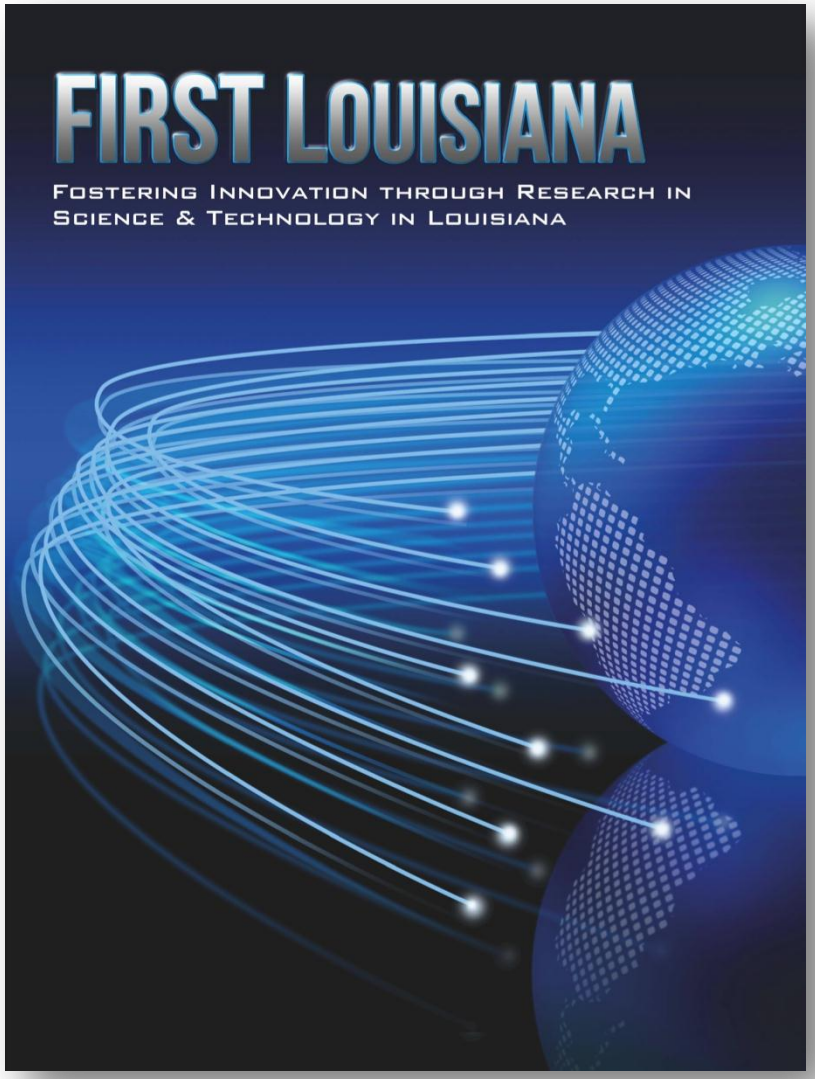
*Louisiana Board of Regents*

Claiborne Building, Baton Rouge, LA

Board of Regents: $10 Million cost-share commitment

# Alignment with State Priorities

## Louisiana S & T Strategy





# Science & Technology Plan:
## Framework and Alignment

**High Growth Target Industry**

Materials & Chemicals | Energy Production | Coastal Resilience | Digital Media | Cyber Security | Biomedical | Bioengineered Solutions

**Core Industry S&T Sectors**

Petrochem | Energy & Environ | Transport, Constr & Mfg | Aerospace | Info Tech & Services | Arts & Media | Agriculture & Bio Prod | Health Care

**Translational Research Domains**

Energy | Environmental | Biomedical | Coastal | Digital | Agricultural

**Core Enabling S&T Research**

Materials Science Nanotechnology | Computational Science Information Technology | Bioscience Biotechnology

**21st Century Building Blocks**

Atoms & Molecules | Bits & Bytes | Nucleic & Amino Acids

**Foundational Sciences**

PHYS | CHEM | MATH | ENGR | COMP SCI | EARTH SCI | AGRI SCI | BIOL | BIOM SCI | ECON & SS

# LA EPSCoR Funding Agencies

| Agency | Federal | BoR Support Fund |
|---|---|---|
| NSF | $98,797,218 | $32,442,036 |
| NASA | 11,436,236 | 10,436,560 |
| NIH | 106,231,410 | 1,148,000 |
| DOE | 8,551,388 | 6,639,590 |
| DOD | 9,533,295 | 2,639,949 |
| EPA | 1,023,649 | 994,542 |
| DOC | 250,000 | 300,000 |
| Total | $235,823,196 | $54,600,677 |

# NSF-EPSCoR Co-Funding

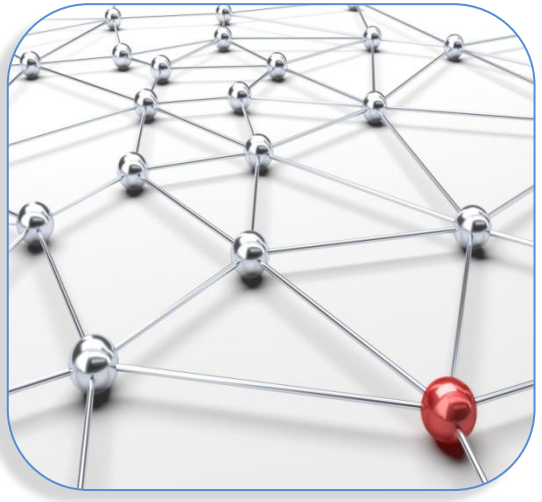
Co-Funding History for Louisiana since 2000

| Year | Total | EPSCoR | No. of Awards |
|---|---|---|---|
| FY 00 | $2,204,762 | $1,059,992 | 9 |
| FY 01 | 4,330,652 | 2,128,636 | 13 |
| FY 02 | 5,823,318 | 2,922,531 | 26 |
| FY 03 | 8,822,162 | 2,995,274 | 18 |
| FY 04 | 14,186,798 | 5,961,313 | 28 |
| FY 05 | 8,134,360 | 2,740,529 | 24 |
| FY 06 | 8,396,096 | 3,058,041 | 26 |
| FY 07 | 10,363,434 | 4,691,849 | 16 |
| FY 08 | 13,810,000 | 3,560,000 | 21 |
| FY 09 | 8,330,000 | 3,440,000 | 16 |
| FY10 | 3,160,000 | 9,300,000 | 18 |
| FY11 | 9,020,000 | 3,362,000 | 25 |
| Total | $96,581,582 | $45,220,165 | 240 |

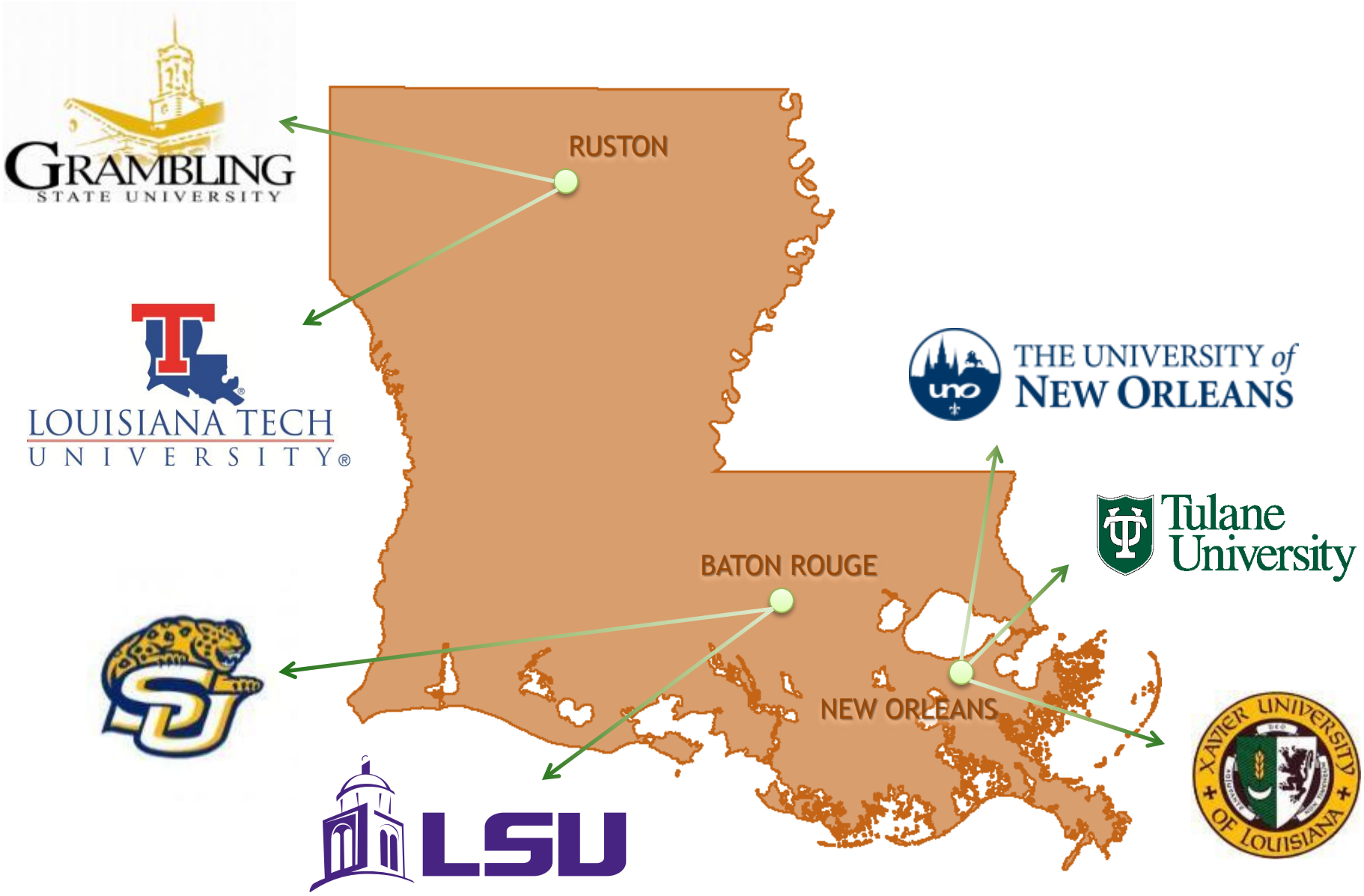
# LA EPSCoR: Catalyst for Collaboration

LA EPSCoR has broken down boundaries between campuses.

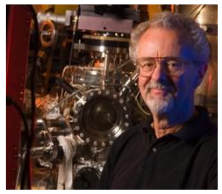
LA EPSCoR is a proven catalyst for achieving increased statewide collaboration and national competitiveness.



# Partnering Institutions



# Participants: 231 partners



**64**
Faculty

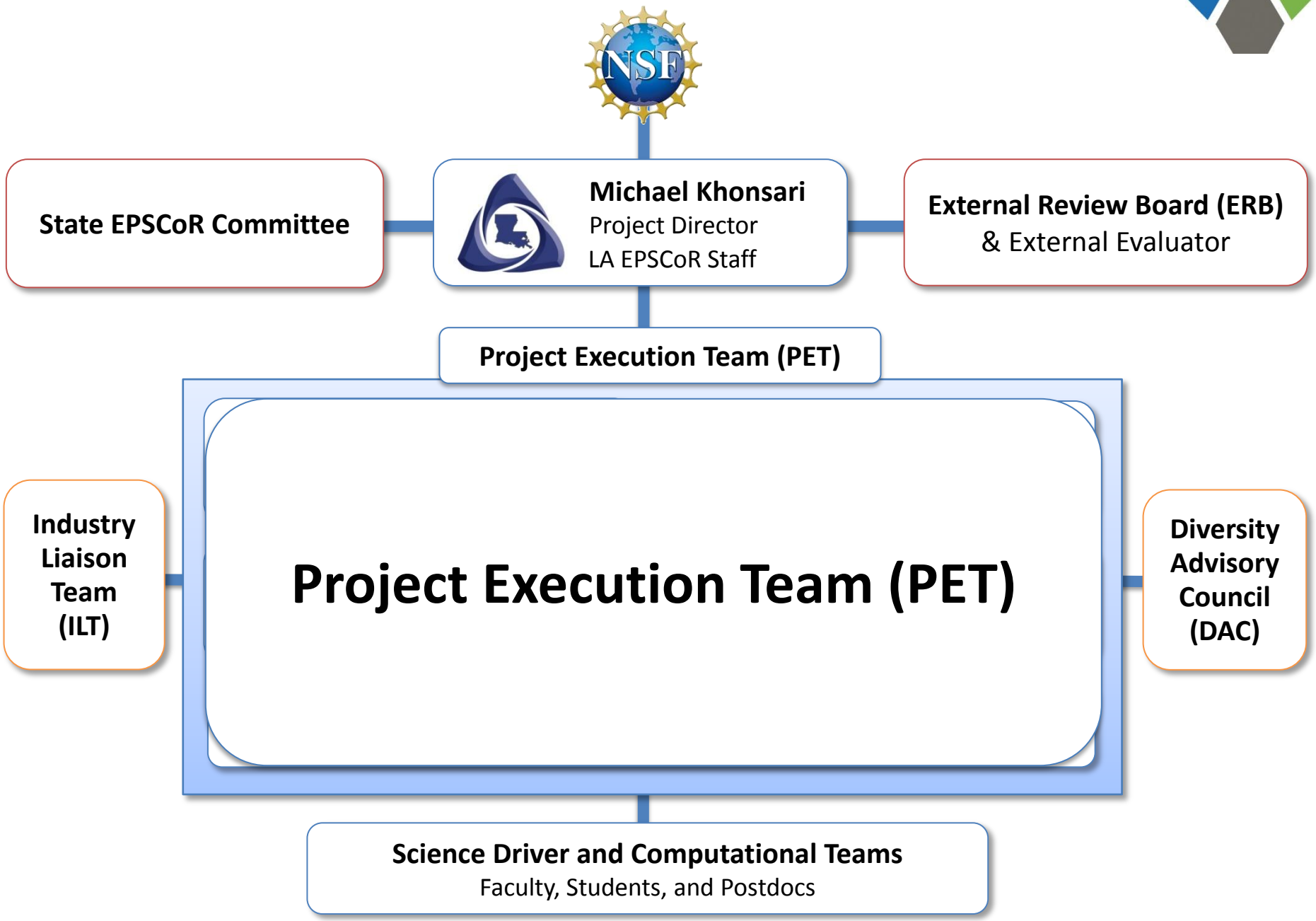
**10**
Post-Doc

**71**
Graduate

**67**
Undergraduate

**19**
Technical / Non-Technical Staff

# RII - Track 1: Management



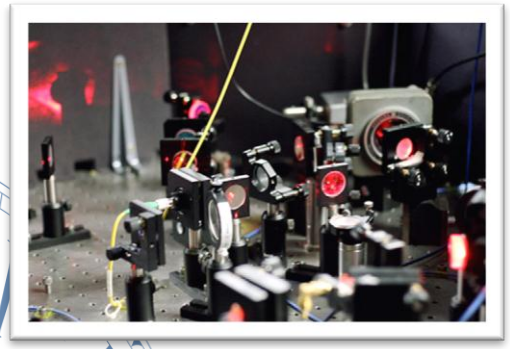
# LA-SiGMA Vision

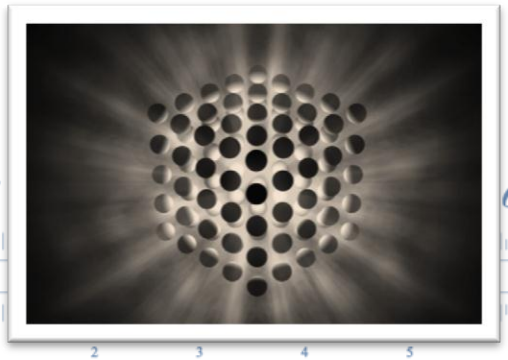
To make transformative advances in materials science research and education through a sustained multi-disciplinary and multi-institutional alliance of researchers.

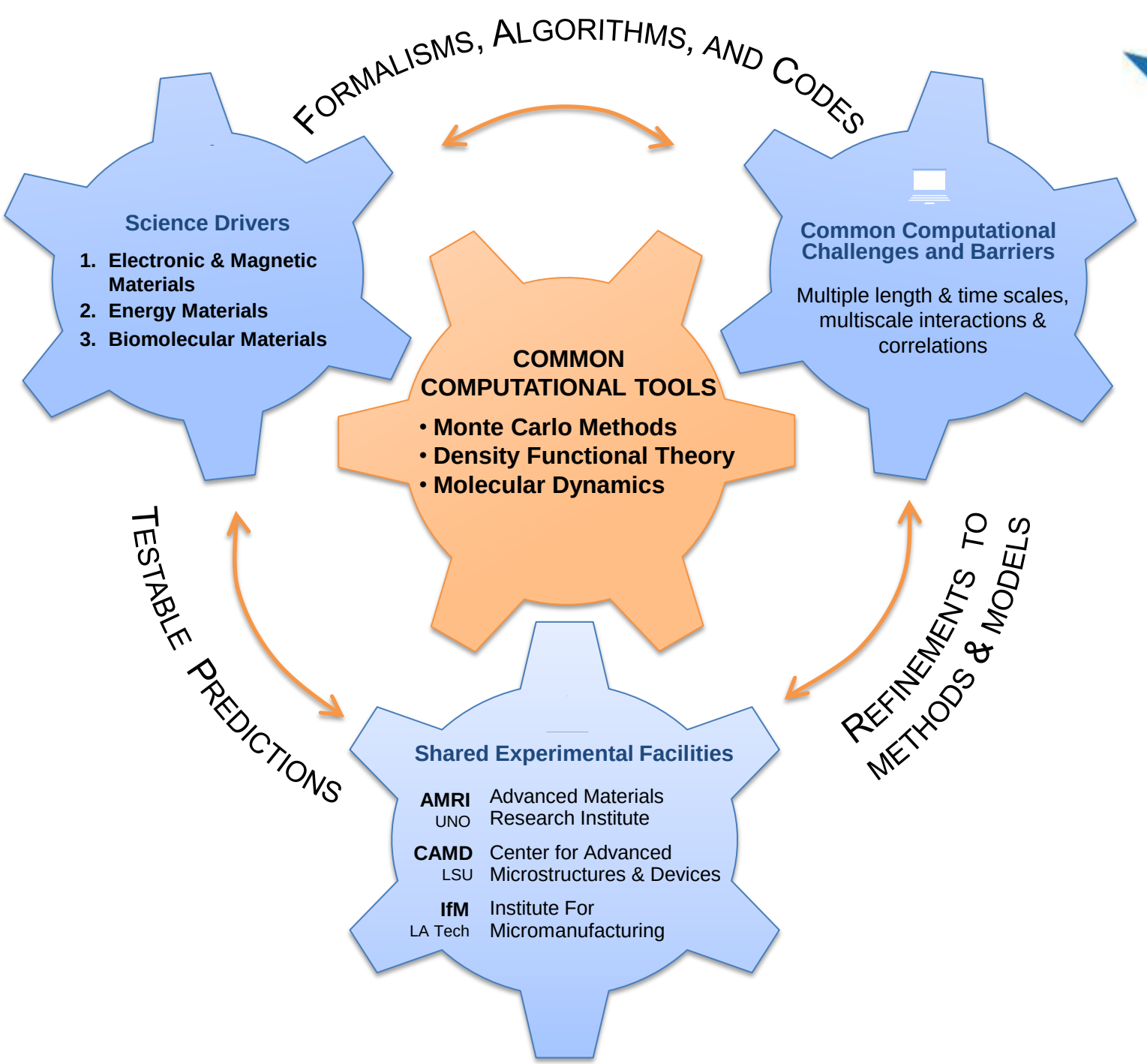
# Scientific and Technological Challenges

Addressing multiscale complex phenomena calls for:

Unprecedented collaboration of computer scientists, applied mathematicians, scientists, and engineers with expertise at each scale from sub-nanometer to millimeters in length and from femtoseconds to several seconds in time.



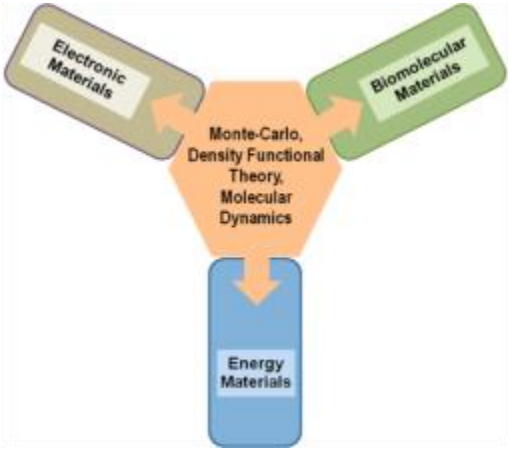



FORMALISMS, ALGORITHMS, AND CODES
Science Drivers
1. Electronic & Magnetic Materials
2. Energy Materials
3. Biomolecular Materials
Common Computational Challenges and Barriers
Multiple length & time scales, multiscale interactions & correlations
COMMON COMPUTATIONAL TOOLS
• Monte Carlo Methods
• Density Functional Theory
• Molecular Dynamics
TESTABLE PREDICTIONS
REFINEMENTS TO METHODS & MODELS
Shared Experimental Facilities
AMRI UNO Advanced Materials Research Institute
CAMD LSU Center for Advanced Microstructures & Devices
IfM LA Tech Institute For Micromanufacturing

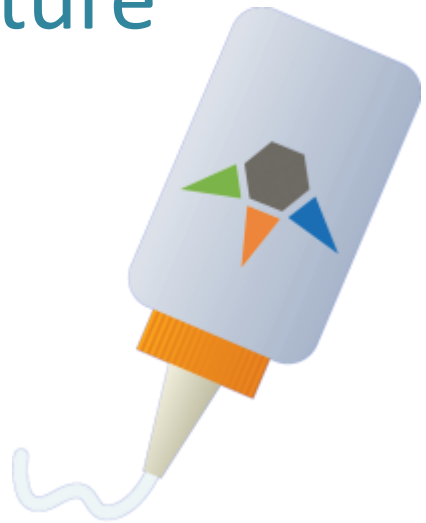
# LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

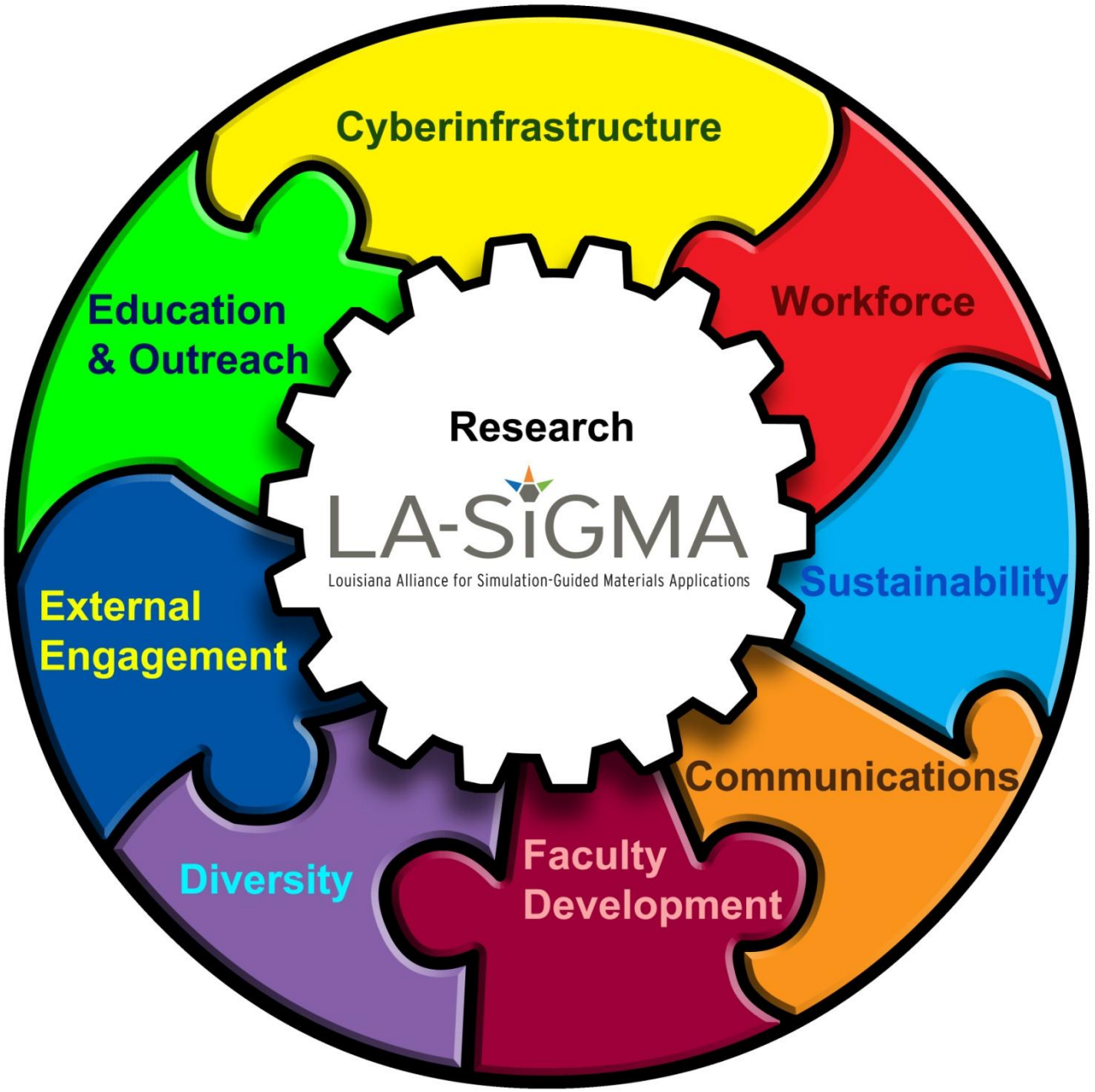
## Computational Teams
## Cybertools/Cyberinfrastructure
## CTCI



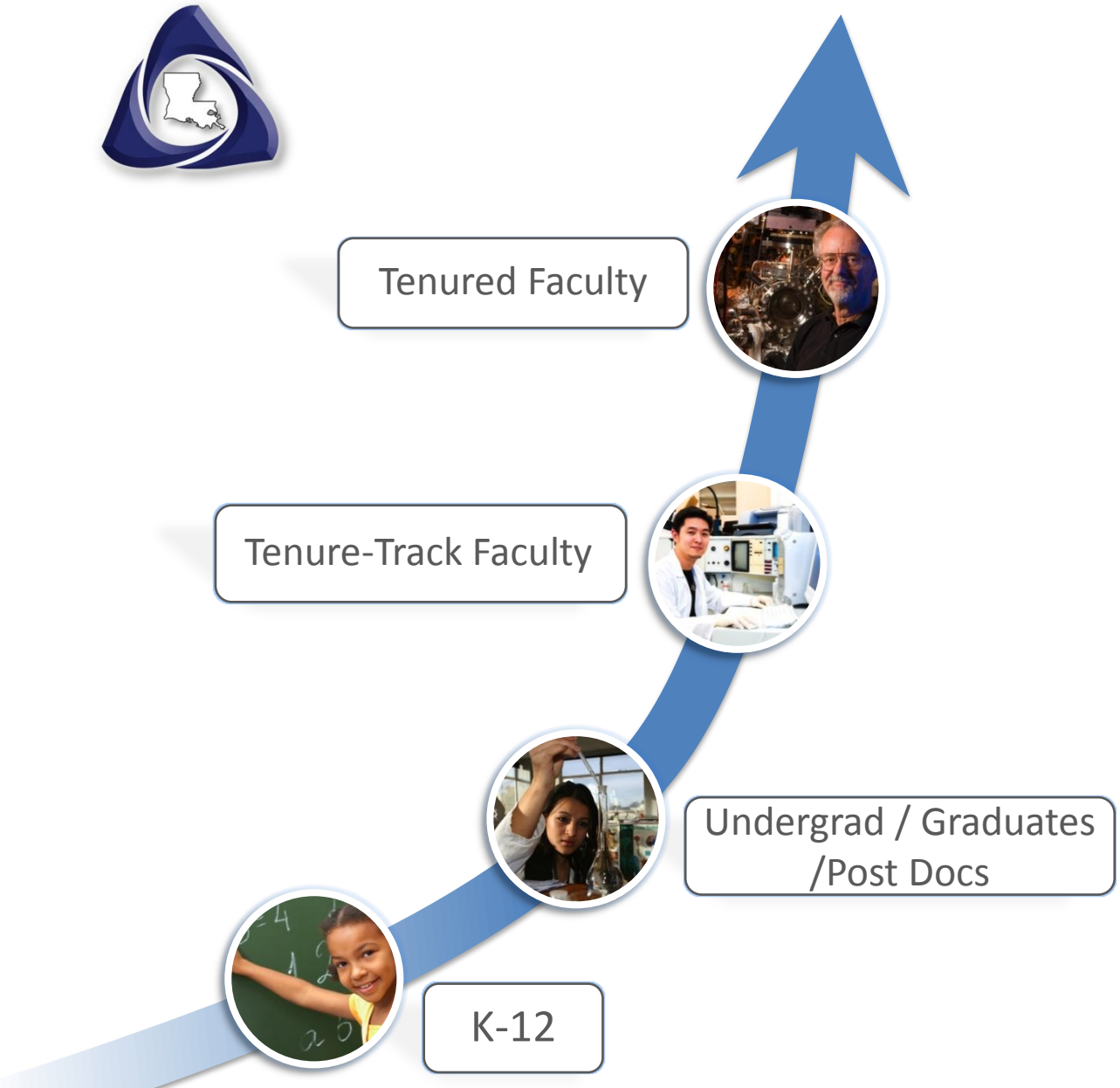

"The glue"



Develop and experimentally validate common computational tools essential for three Science Drivers.


Cyberinfrastructure
Workforce
Education
& Outreach
Research
LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications
Sustainability
External
Engagement
Communications
Diversity
Faculty
Development

# Traveling the STEM Pipeline




## Programs

LINK
Planning
Grants
Pfund
SBIR/STTR
TGEF
OPT-IN

SURE
REU
LINK

SoS

# LA-SiGMA: Year 2

**96**
Proposals Submitted

**33**
Proposals Awarded

**39**
Publications


**38.5 Million**
External Funding

# LA-SiGMA:
# Year 1 and Year 2

**144**
Proposals Submitted

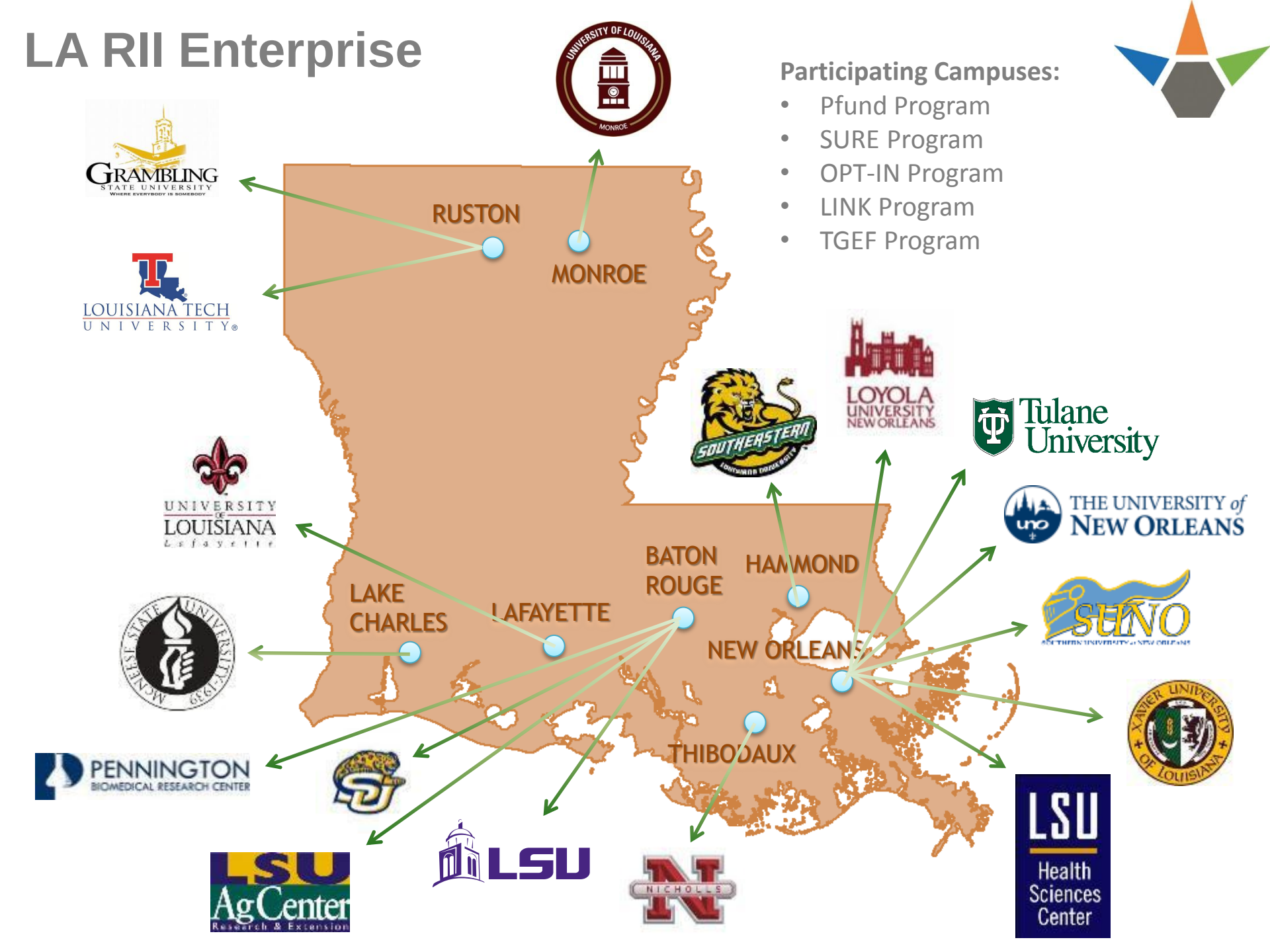
**63**
Proposals Awarded

**83**
Publications


**64.6 Million**
External Funding

**1**
Patents

# LA RII Enterprise

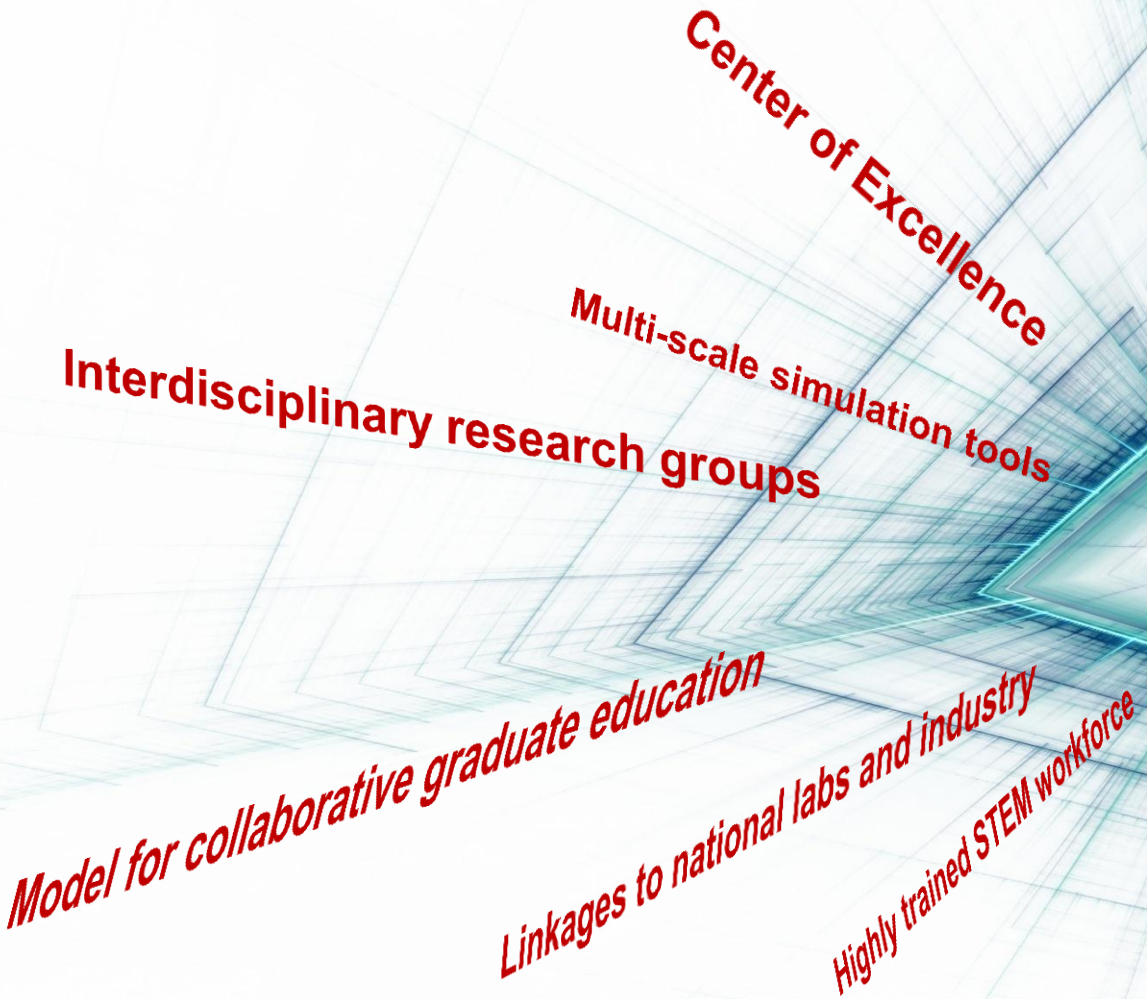



**Participating Campuses:**

- Pfund Program
- SURE Program
- OPT-IN Program
- LINK Program
- TGEF Program

# LA-SiGMA Present and Future

Collectively we are on track to make transformative advances in materials science research and education



# Agenda

# **Session 1:** Science Drivers & CTCT

| **Science Drivers (SD) and CyberTools and CyberInfrastructure Group (CTCI)** | |
|---|---|
| **8:20 – 8:45** | Electronic and Magnetic Materials (Bagayoko and Perdew) |
| **8:45 – 9:10** | Materials for Energy storage and Generation (Pratt and Mainardi) |
| **9:10 – 9:35** | Biomolecular Materials (Ashbaugh and Nikitopoulos) |
| **9:35 – 10:00** | Computational Tools for Multiscale Simulations (Bishop, Yun, Jarrell) |

# Session 2:
# Assessment and Broader Impacts

| | |
|---|---|
| **10:25 - 10:45** | Diversity and Workforce Development **(Moreno and Hall)** |
| **10:45 - 11:00** | External Engagement and Sustainability (Pesika and Domingue) |
| **11:00 - 11:15** | Industrial Liaison (Whittenburg and Cruthirds)<br>Jeff Lynn (Louisiana Economic Development) |
| **11:15 - 12:00** | Presentations by invited recipients of EPSCoR awards: Carlos Montes (LA Tech); Laura Schrader (Tulane); Mark Merchant (McNeese) |

# **Session 3:** DMP, Training and Evaluation

| | |
|---|---|
| **12:00 – 2:30** | **Lunch and poster session** |
| **2:30 – 2:45** | Data Management Plan (Joel Tohline and Lawrence Pratt) |
| **2:45 – 3:00** | Graduate Student Retreat (Chinedu Ekuma) |
| **3:00 – 3:15** | FIRST Training Program (Cynthia Sisson) |
| **3:15 – 3:30** | Evaluation and Assessment (Cindi Dunn) |

# **Session 4:** Planning

| Planning Session | |
|---|---|
| 3:45 – 4:45 | Simultaneous sessions:<br>ERB Deliberations<br>DAC Deliberations<br>LA-SiGMA members: Breakouts |
| 4:45 – 5:00 | DAC and ERB debriefing to LA-SiGMA |
| 5:00 | Concluding Remarks (Khonsari) |