LA-SiGMA

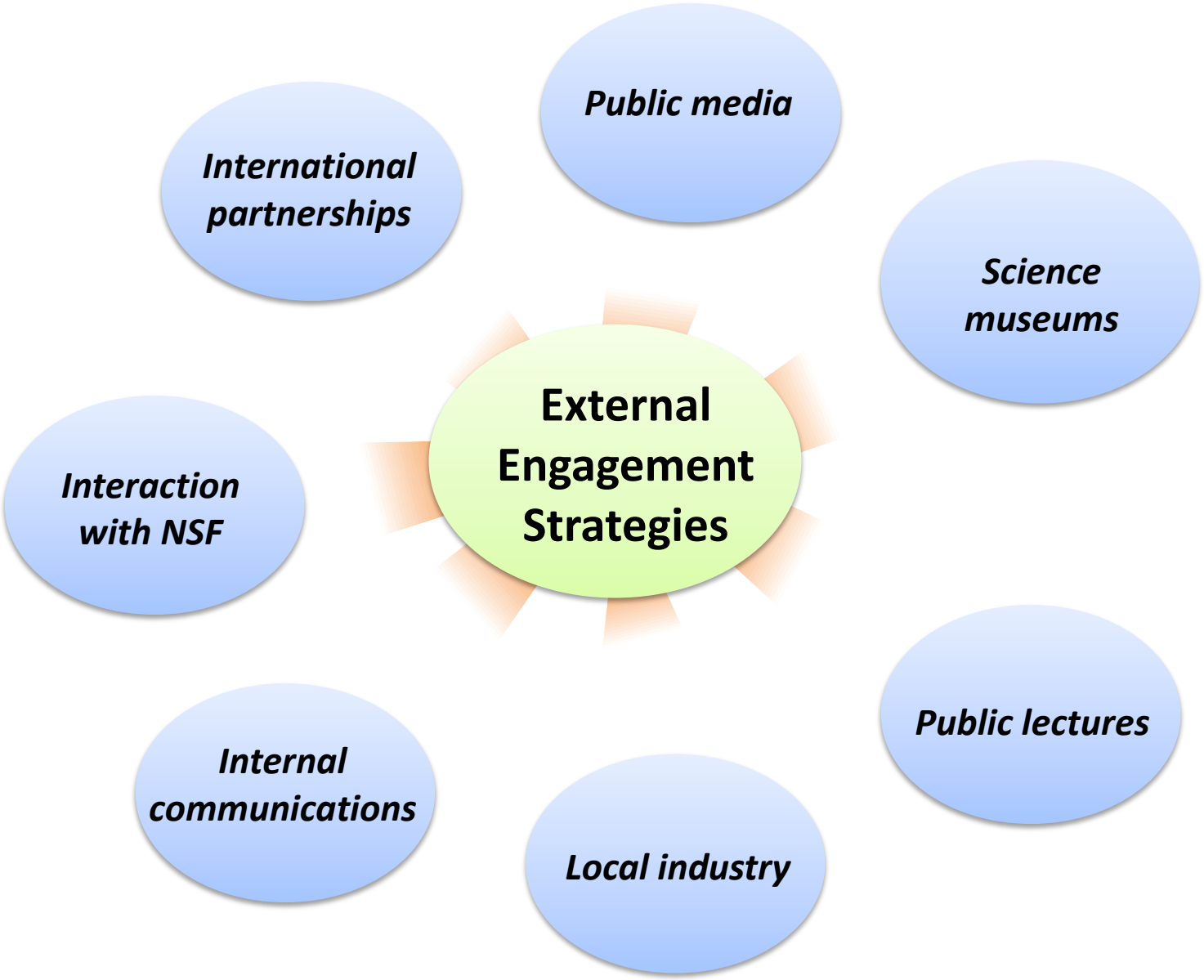
Louisiana Alliance for Simulation-Guided Materials Applications

External Engagement

Noshir Pesika

LA-SiGMA will provide for efficient collection and dissemination of information between participants, the K-12 community, two-year colleges, and the general public.

External Engagement Strategies



External Engagement Milestones

Strategies	Y1	Y2	Y3	Y4	Y5	
Leverage multiple avenues to engage the general public.	X	X	X	X	X	*On Track**
Create a web portal for distribution of project deliverables.	X	X	X	X	X	*On Track*
Create a repository and version control system for code development and distribution.	X	X	X	X	X	*On Track*
Leverage cyberinfrastructure to facilitate communication.	X	X	X	X	X	*On Track**
Use Newsletter/Brochures/Highlights to publicize Alliance activities.	X	X	X	X	X	*On Track*
Create formal mechanisms for engagement with NSF.	X	X	X	X	X	*On Track*
Establish new national and international collaborations.	X	X	X	X	X	*On Track*
Create mechanisms for internal communications.	X	X	X	X	X	*On Track*

*Pending LPB appearance and HD video conferencing equipment purchase.

Mitigation plan: Working with LPB for feature, HD standards being finalized.

Engaging the Public

- ✓ Nanodays in Baton Rouge, March 24 and 31, 2012
- ✓ Public talks by DiTusa & Sprunger

- ✓ SciPort Discovery Center, Shreveport, February 21,2012

- ✓ Super Science Saturday, Baton Rouge, October 15, 2011

- ✓ NSF/LA EPSCoR sponsored workshop: Science: Becoming the Messenger, November 17, 2011

Industrial Collaborations

- ✓ Active ILT
- ✓ La Tech researchers continue to build their relationship with Carbon Capture Energy Technologies and Avoyelles Energy
- ✓ Xavier working with Absorption Systems, Inc of Philadelphia
- ✓ UNO working with Vertex Pharmaceuticals
- ✓ LSU working with Albemarle Corporation

Website

- ✓ Tracking is enabled, but not yet explored

Facebook

Leveraging LONI Facilities

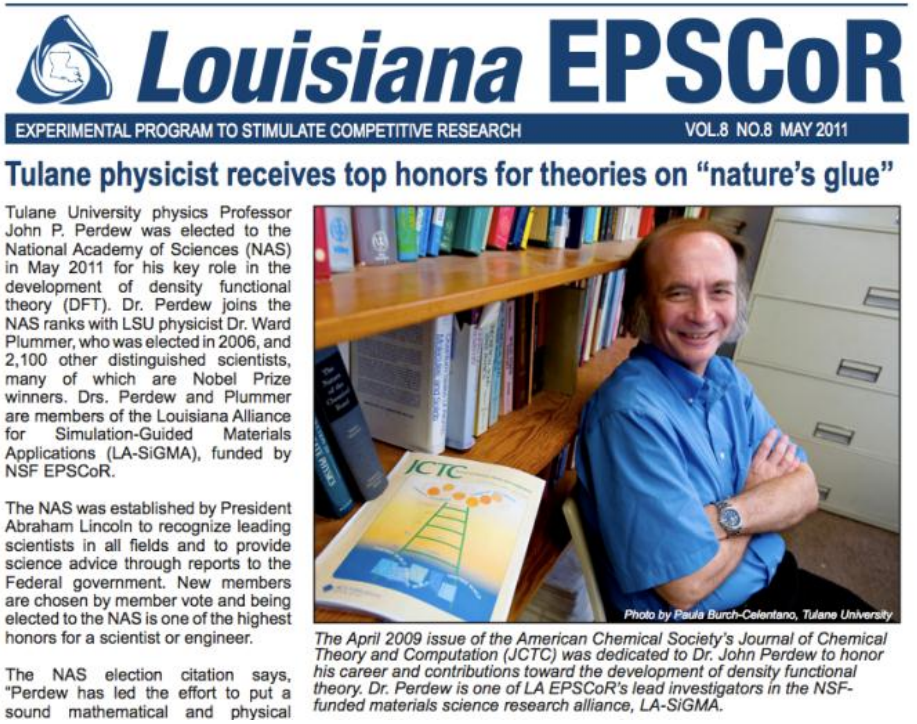
- ✓ LA-SiGMA investigating **collaborative** (LONI, BoR) solutions for ***HD*** synchronous video, lecture/seminar ***capture, and digitization***
- ✓ LONI will help fund the HD solution
- ✓ Technical contacts and EEWD members discussing details

Newsletters and Highlights

- ✓ Speaking of Science speakers
- ✓ 8 faculty, LA Tech (1), LSU (1), Xavier (3), UNO(2), Tulane (1)

NSF Highlights

LA-SiGMA NSF Highlights 2011		
Optimized Simulation Model for the Quantitative Description of Hydrophobic Hydration	H. Ashbaugh	(PDF)
A Mathematical Pathway to Predictive Calculations of Properties of Materials	D. Bagayoko	(PDF)
Temporal Pattern Discovery in High-throughput Data Domain	S. Dua	(PDF)
Thermodynamics Indicate Iron Oxide Clusters' Reactions with Molecular Precursors are Favorable	R.Hall	(PDF)
Copper Oxide-Clusters Model of Persistent Free Radical Formation: A computational Approach	R. Hall	(PDF)
Interdisciplinary Physics/Computer Engineering Collaboration Speeds Many-Body Codes to 30,000 Processors	M. Jarrell, J. Moreno, J. Ramanujam	(PDF)
Computer Hard Drives Made with Single-Molecule Magnets Promise Very High Information Density	V. Kolesnichenko	(PDF)
Atomistic Simulations Show Proof of Concept for a Novel DNA Sequencing Technology	D. Moldovan	(PDF)
Scale-Bridging Simulator for Non-Equilibrium Processes Involving BioMaterials	D. Nikitopoulos	(PDF)
Research on Thermoelectric Properties in Doped C_{60}	G. Zhao	(PDF)



Louisiana EPSCoR

EXPERIMENTAL PROGRAM TO STIMULATE COMPETITIVE RESEARCH VOL.8 NO.8 MAY 2011

Tulane physicist receives top honors for theories on "nature's glue"

Tulane University physics Professor John P. Perdew was elected to the National Academy of Sciences (NAS) in May 2011 for his key role in the development of density functional theory (DFT). Dr. Perdew joins the NAS ranks with LSU physicist Dr. Ward Plummer, who was elected in 2006, and 2,100 other distinguished scientists, many of which are Nobel Prize winners. Drs. Perdew and Plummer are members of the Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA), funded by NSF EPSCoR.

The NAS was established by President Abraham Lincoln to recognize leading scientists in all fields and to provide science advice through reports to the Federal government. New members are chosen by member vote and being elected to the NAS is one of the highest honors for a scientist or engineer.

The NAS election citation says, "Perdew has led the effort to put a sound mathematical and physical

Photo by Paula Burch-Celentano, Tulane University

The April 2009 issue of the American Chemical Society's Journal of Chemical Theory and Computation (JCTC) was dedicated to Dr. John Perdew to honor his career and contributions toward the development of density functional theory. Dr. Perdew is one of LA EPSCoR's lead investigators in the NSF-funded materials science research alliance, LA-SiGMA.

- ✓ May 2011 LA EPSCoR newsletter (published October 2011)

Newsletters and Highlights

✓ LA-SiGMA highlighted in Fall 2011 LSU Research Magazine

A Material World

LSU Materials Science Group Lands Major Grant

Ashley Berthelot

With technology driving the global economy, the workforce and our day-to-day lives, many believe that materials science—the study and design of custom materials with task-specific properties—is the key to our future. In light of this, LSU has made materials science a focus of interdisciplinary study on campus for several years, and recently, researchers had their efforts paid back by the millions.

Faculty at LSU, together with scientists at universities across Louisiana, received one of the state's largest ever grants from the National Science Foundation, or NSF, to form the Louisiana Alliance for Simulation-Guided

James Madden teaches LA-SiGMA-supported teacher-students during the

implementation on present and next generation supercomputers, and educating the next generation of a highly skilled workforce of materials scientists and engineers. The group has made significant progress toward these objectives. In fact, during the summer of 2011, LA-SiGMA and CCT hosted more than 20 undergraduate and high school students at LSU in a Research Experience for Undergraduates, or REU, program, offering the opportunity for a cutting-edge research experience with LSU faculty.

LA-SiGMA program objectives include educating the next generation of highly skilled materials

LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Elements of LA-SiGMA will include:

- an education plan that includes new materials science graduate courses delivered across the state
- well-developed relationships between research universities, two-year colleges and the K-12 community through ongoing outreach efforts
- strong partnerships between Historically

Internal Communications

Leverage cyberinfrastructure, video-conferencing, collaboration tools, web portal, all-hands meetings.

- ✓ Monthly seminars
- ✓ Monthly meetings of the SD and CTCI teams

LI/LA-SiGMA Seminar Series

The LONI Institute/LA-SiGMA seminar series started in September 2010 and is designed to provide a strong platform for interactions between various elements of the Loni Institute and LA-SiGMA . It is also expected to improve the general research atmosphere, and provide

February 2012		
Date/Time	*Speaker*	*Title*
Feb 15 10 a.m. Live at LSU	Karol Kowalski	"Coupled-Cluster and Configuration-Interaction Methods in Terms That Even Physicist can Understand"
Feb 24 3:30 p.m. Live at LSU	Peter Nordlander	"Plasmonic Nanostructures: Artificial Molecules"
March 2012		
March 13 11 a.m. Live at LA Tech	Ras Pandey	"Multigrain Computational Approach to Morphing Nanostructures."
March 21 10 a.m. Live at LSU	Kieron Burke	TBA
April 2012		
April 11 10 a.m. Live at LSU	Vaclav Janis	TBA

Schedule | FALL 2011

September 2011		
Date/Time	*Speaker*	*Title*
TBA		

National and International Partnerships

LA-SiGMA International Computational Materials Science Seminar Series

Schedule

The slides and videos for the previous seminars can be downloaded via the links below (For the video, it requires the recording player from EVO)

November 2011

Date/Time	*Speaker*	*Title*
Nov 2 10 a.m. (EST)	Bayo Lau, Columbia University	An Efficient Numerical Approach to Model of 2D S=1/2 Antiferromagnet and Doped CuO2 Planes Download Slides Download Video

December 2011

Date/Time	*Speaker*	*Title*
Dec 14 9 a.m. (CST)	Tom Berlijn, Brookhaven National Laboratory	Wannier Function Based First Principles Methods for Disordered Systems Download Slides Download Video

- ✓ International Symposium Series

Target: National and International Partnerships

- ✓ LSU has SAVI whitepaper at NSF, targeting Africa in addition to existing collaborations
- ✓ PNNL NWCHEM center proposal
- ✓ New collaboration between La Tech and Florida A&M focusing on iron oxide nanoparticles
- ✓ Xavier collaborating with Institute for Physical Science, Kiev and University of Tennessee Space Institute

- ✓ SUBR developing collaborations with Turkey, LANL, and Lehigh
- ✓ UNO has collaborations with Cincinnati and Sandia
- ✓ LSU collaborates with Karlsruhe Institute of Technology and Grenoble
- ✓ LSU collaborates with APS/ANL on phase contrast imaging
- ✓ LSU collaborating with Brazil

LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Thank you

External Engagement

Activity	Number
Public Lectures	0
Appearance on local/statewide TV or radio	0
Advised a science museum	0
Delivered a lecture to an industry	1
Used web portal to distribute project deliverables	1
Uploaded codes to the repository	0
Contributed a highlight to the EPSCoR newsletter	0
Submitted a research highlight	0
Used video conferencing	1
Had a LA-SiGMA story picked up by national/regional press	0
Participated in biannual meeting	2
Served as a speaker for SoS	1