Report of the External Review Board
Louisiana's NSF EPSCoR Research Infrastructure Improvement (RII) Award
August 5-6, 2011

The External Review Board (ERB) for Louisiana's EPSCoR Research Infrastructure Improvement Award met in Baton Rouge, Louisiana on August 5 and 6 to assess the progress of the project and to recommend possible improvements to the program for consideration by the leadership. ERB members present included Dr. Vincent McKoy (Chair), Professor of Chemistry, California Institute of California; Dr. William Lester, Professor of Chemistry, University of California (Berkeley); Dr. Harold Silverman, Professor of Biological Sciences and Dean Emeritus, Louisiana State University and Senior Associate-Provost, State University of New York System (Retired); and Dr. Susan Sinnott, Professor of Materials Science, University of Florida. One member of the ERB, Dr. Valerie Taylor, Professor of Computer Science, Texas A&M University, was unable to attend due to a prior commitment. McKoy and Silverman served on the ERC for Louisiana's previous RII award and Sinnott served on a "mock" review team that reviewed the proposal for the current RII program prior to its submission to NSF. Members of Louisiana's EPSCoR Committee, including Dr. Kerry Davidson, Deputy Commissioner for Sponsored Programs for Louisiana's Board of Regents, also participated in the meeting. The meeting was held concurrently with the annual meetings of the Diversity Advisory Committee and the External Evaluation Committee for this award and in conjunction with the biannual statewide all-hands meeting with researchers, students, and administrators. The ERB participated fully in LA EPSCoR Symposium, which included presentations on the scientific progress of the project, outreach and educational activities, diversity initiatives, and industrial interactions, as well as a poster session, primarily hosted by graduate students and postdoctoral scholars.

On August 6 the ERB also heard presentations on the progress of the Cyber Connectivity (C-2) project, an award intended to extend LONI's (Louisiana Optical Network Initiative) high-bandwidth optical network into Xavier University of Louisiana. This extension will close a gap in the existing network and will facilitate research collaborations between faculty and students at Xavier University and the other computational and experimental groups in Louisiana, as well as partnerships with major institutions nationally.

Summary

The ERB was impressed by the compelling goals and vision of this initiative to transform research and education in computational materials science throughout Louisiana. This effort, which seeks to develop common computational tools for the study of multiscale phenomena in three areas of materials science with potentially significant technological and economic impact, speaks clearly and deliberately to the strategic leveraging of prior investments in cyberinfrastructure and cybertool development in Louisiana. The three Science Drivers or thrusts of the initiative: (i) correlated electronic materials, (ii) energy materials, and (iii) biomolecular materials, should benefit from the synergisms of the

common set of computational challenges. The close integration of the theoretical, computational, and experimental scientists has substantial merit and could greatly facilitate the experimental validation of the computational approaches. Such validation of computational approaches is much needed and could potentially transform the utility of simulation-guided materials science. Inclusion of two members of the National Academy of Sciences in the leadership of the Science Drivers speak well of the scientific strengths of the projects and of the teams. A team approach to leveraging advances in computational tools and methodologies was evident in the written materials provided and in the results presented. The progress report and other written materials were very strong and well assembled.

The ERB commends the leadership for the responsive and effective management structure it has put in place. The ERB was pleased with the effort to develop both traditional and online courses in computational material sciences, not only at the graduate and international levels but also for undergraduate and K-12 students, and commends the REU (Research Experiences for Undergraduates) and SURE (Supervised Undergraduate Research Experiences) programs for their efforts to specifically impact underrepresented minorities and women. Industrial interactions are also a strong component of the effort as evidenced by the active participation in the meeting by a team from the Governor's Workforce Development Office. The ERB believes that these interactions hold much potential for meaningful growth. In summary, while our overall findings are that this is an impressive beginning to an appropriately ambitious project, we will offer suggestions in this report that might lead to even further improvement in the program.

The Science Drivers

The research thrust of the project is structured around three Science Driver areas: (i) correlated electronic materials, (ii) energy materials, and (iii) biomolecular materials. Researchers belong to one or more of the Science Driver teams as well as to the computational team that include experts to help translate formalisms into algorithms and efficient cybertools running on high-performance computing platforms. This structure should provide for optimum coupling between the materials scientists and the cybertool experts. The team approach to addressing the scientific challenges of this ambitious project, both from a perspective of institutions and scientific disciplines, seems to be developing well as was evidenced in the written progress reports and the poster sessions. Across the numerous scientific foci, computational and material scientists were clearly having productive interactions. This was particularly so for Science Driver 1 with the goal of taking simulations of electronic materials to the next level by extending the methods that are currently used such as the Local Density and Dynamical Mean Field Approximations to much larger length scales. A key goal here would be for these researchers to model accurately strongly correlated materials on national leadership class supercomputers for the first time. Highly correlated electron systems can enable new devices by enhancing their sensitivity to applied fields, and the success of this effort can be transformative. The goals and proposed simulations, as well as algorithmic developments,

for this science driver were clearly articulated. The effort is at the cutting edge and the progress to date was clearly summarized.

The goal of Science Driver 2 is to develop and apply novel density functional theory formulations, reactive and transferable force fields, and high-performance Monte Carlo and molecular dynamics methods to enable multiscale (both length and time) simulations of materials for storage and generation of energy. In contrast to the clarity of the goals and progress that characterized the presentations on Science Driver 1, the discussion of the force field simulations and requisite technical details were less transparent. The exact contributions, as well as their potential novelty, were not well articulated in the oral presentations on this Science Driver. How this effort is actually leveraging advances in Science Driver 1 should be more clearly defined in order to make the cohesion of the goals of the project more transparent. Comparison of the effort with what others, nationally and internationally, are doing in multiscale modeling and in the development of force fields for similar applications would have put this effort in better perspective. More context and greater justification would have improved this presentation. Likewise, the novelty of the goals of Science Driver 3 to develop new biomolecular materials for the encapsulation, delivery, and release of therapeutics to targeted tissues became noticeably more evident to the ERC during the preview of the reverse site presentation to NSF than during the presentations at the all-hands meeting. The ERB believes it is critical that presentations crisply outline the novel outcomes expected of each of the Science Drivers as well as situate the potential contributions and their impact in the context of ongoing work in the field. The ERB is, however, of the opinion that significant progress is being made and these comments are intended to encourage the researchers to be more cognizant of these issues in future presentations.

The poster session offered the ERB the opportunity to interact with students and postdoctoral scholars and provided a window on the scientific projects and specific approaches that was complementary to the overview talks. The scientific collaborations across the program were clearly evident in the poster session where one could see students with mentors from institutions or departments other than their own. The ERB members appreciated the high level of enthusiasm of the poster presenters. Unfortunately, the quality of many of the poster presentations was more mixed than the ERB expected. Some were truly excellent with well-prepared and articulated by informed student presenters who were clearly contributing to the success of the effort. However, others seem less integrated into the overall research objectives than anticipated for an integrated collaboration. A firm grasp of the background, goals, and the requisite techniques underpinning an effort should be expected of all students and collaborators involved in a project. The diversity of the students presenting the posters was evident and a strength of the project. In fact, the award for the best poster went to students from underrepresented minorities who will present their posters at the upcoming national EPSCoR meeting in Idaho.

Computational Tools for Multiscale Simulations

The overview of the cybertools and cyberinfrastructure for the proposed simulations highlighted Louisiana's prior investments in computational resources through LONI and CCT as well as strategies for advancing the simulations to expanded computer architectures and to DOE's Leadership Computing Facilities. There is much emphasis on shifting the computations from CPU's to GPU's. The ERB commends the LA-SiGMA team for its resourcefulness and the State for its infrastructural investments but must express some concern for developments that could impede progress. While the State has assembled an excellent team of scientists, particularly those associated with Science Driver 1, it has lost the cadre of scientists who were primarily responsible for the initial strategy for marshalling the cyberinfrastructure to address significant computational scientific challenges. These were primarily computational scientists who could be considered the base upon which the present RII effort sits. Recently, Jha, Sterling, Allen, Kosar, Chen, and Iyengar and numerous staff have left LSU. Losing such a base is not consistent with the impressive plans outlined for the LA-SiGMA project. The ERB encourages the leadership to rebuild the core computational science and engineering faculty to the extent possible.

Evaluation and Assessment

The principal investigator and the co-principal investigators and their team have clearly invested significant effort in developing a strategic plan that was submitted and then resubmitted with revisions in response to comments by NSF. The external evaluator, Cindy Dunn, of Kansas State University and her colleagues have collected pre-award data, created a logic model, and collected data over the first year of this award. Their efforts seem robust and comprehensive and should provide an insightful evaluation and assessment of progress, as well as an opportunity to make adjustments for improvement as the program progresses. The Diversity Council met during the review and has provided recommendations to improve pertinent activities based on their observations to date.

External Engagement

There is a clear plan for external engagement that aims to provide a well-prepared and competent workforce and an educated public. The ongoing effort by the LA-SiGMA to engage Louisiana Public Broadcasting to produce a program in their series "The State Where We Are" could be a very effective vehicle for communicating scientific advances and discoveries to the general public. Such a program could be featured repeatedly throughout the State and is an excellent way to reach citizens of all ages with an interest in advancing science in Louisiana. It is politically visible and reaches the leadership in the community and industry. The tried and proven "Speaking of Science" series reaches out to the K-12 constituency and should complement many of the other proposed initiatives for external engagement. Websites and FaceBook accounts have been established and there have been numerous meetings with industry leadership. Leveraging partnerships with the national laboratories should also be effective in promoting collaborations that should benefit both faculty and students.

Education and Outreach

The education and human resources development elements of the program, as well as the outreach strategy, being put in place are varied, robust, and promising. Some outreach programs aimed at K-12 levels statewide are new while others are continuations of proven programs initiated under prior RII awards. Tulane is seeking a candidate to fill an endowed chair in materials sciences and the College of Science at LSU apparently plans to hire a scientist with proven expertise in molecular dynamics to drive the development of the next generation of algorithms for molecular dynamics simulations. The ER**B** also encourages the leadership to consider recruitment of a computational chemist with expertise in modern electronic structure methods. Such an appointment could significantly enhance the capacity of the teams to address core needs of Science Driver 1 (electronic and magnetic materials), but especially of Science Driver 2 (materials for energy storage and generation) and/or Science Driver (biomolecular materials). Much of the $10M in matching funds from the Board of Regents is being used to support education and outreach efforts. Traditional and web-based courses focusing on cutting-edge computational methods and tools for simulations also appear quite strong. Outreach programs providing opportunities for students and faculty to interact with scientists at national laboratories and to encourage collaborations between scientists in industry and those working in the LA-SiGMA project have been put in place. Resources available to match funding from industry in support of internships and scientific initiatives have the potential to stimulate sustainable collaborations with industrial partners and to position scientists in the program to exploit the impressive cyberinfrastructure coming on line at the national laboratories. The ERB encourages the leadership to explore leveraging possible collaborations with the LIGO educational facilities in its K-12 outreach effort. Such collaborations would have clear national implications and could become a signature outreach effort of this program.

An outreach effort with potentially high impact is also being explored and developed with Indian scientists on Science Driver 1 as its primary focus. This effort is both timely and appropriate in view of the recent agreements between the US and India to enhance scientific collaboration. Opportunities with the SciDAC and INCITE programs of the Department of Energy are also being sought. All of these efforts add scientific and educational value to the program but the ERB advises the leadership to be sure that the overall focus and goals of the initiative are maintained. The ERB also advises that caution should be exercised to avoid any overextension of the core scientific leadership while pursuing these opportunities.

Relationships with Industry

Industrial interactions are a strong component of the effort and technology transfer is a priority for the Science Driver teams. A building under construction on the LSU campus with funds from EA Sports and the State to house the Center for Computational Technology (CCT) is a success story of prior interactions with industry that have been successful. The media-based use of technology and the continued evolution of CCT also point to the success of previous EPSCoR efforts. The ERB believes that awarding grants to

link individual investigators and students to specific companies (with matching funds) could potentially result in similar examples of success and speak to the seriousness of these efforts. The LA-SiGMA leadership has established a committee of technology transfer officers to work specifically on linking the needs of technology-based industries with the research effort and expertise being developed. The ERB commends the establishment of an Industrial Liaison Team to identify industry and government partners who can participate in the ongoing research projects and exploit the tools and other outcomes of the research effort. The presentation by a representative from the office for Louisiana Economic Development (LED) within the Department of Labor at the all-hands meeting bodes well for the continued development of industrial ties within the State and for meaningful economic impact of LA-SiGMA.

Management Structure

The ERB commends the leadership and project participants for the organizational structure and progress that were evident just a year into the effort. A responsive and effective management structure has clearly been put in place and seems to be functioning well. This ambitious project requires a serious commitment to collaboration among numerous institutions, efficient use of shared resources, and a capacity to accommodate institutions with varied constraints and goals. Often the most challenging stage of such a complex project is getting it off the ground. The leadership skills of the teams were evident in the progress reported in the written materials and all-hands presentations. Those who have participated in previous RIIs, particularly Mike Khonsari and Les Guice, have demonstrated the requisite skills and patience, while Mark Jarrell and Randy Hall have come up to speed quickly and adjusted to the complexity of the EPSCoR program. The scientific progress to date speaks to the potential of the project to make cutting-edge strides in understanding the properties of a range of materials. The effort has the capacity to develop and sustain a more diverse research community in Louisiana. The effort builds on prior projects that have developed leaders for Louisiana and the country. The ERB could not overemphasize the importance of continuity of effort and commends all participants for their efforts to date. The ERB is above all mindful of the loss of key faculty and hopes that this project provides opportunities to repair and replace lost expertise in computational/computer science. Expertise in simulation is essential to achieve the goals of this RII and the leadership of LA-SiGMA should be attentive to opportunities to rebuild this expertise at every opportunity.