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Tooling in Cyberspace

The following is the third in a series on the recent $9 million National Science Foundation EPSCoR grant to a team of researchers from nine Louisiana universities to develop CyberTools that will enable researchers to make significant advances in science and engineering. The participating institutions are Louisiana State University, LSU Health Sciences Center-New Orleans, Louisiana Tech University, Southern University-Baton Rouge, Tulane University, Tulane University Health Sciences Center, University of Louisiana-Lafayette, University of New Orleans, and Xavier University. With matching funds of $3 million from the Board of Regents Support Fund and $3.2 million from the participating institutions, the total of the three-year award is over $15.2 million.

There are tools and then there are CyberTools. They don't fit neatly in a kit or a box. You can't even touch them. In the right hands, however, they create the infrastructure required to support current and future discoveries in science and engineering.

The innovative collection of cyberservices and computational toolkits being developed by the NSF EPSCoR Research Infrastructure Improvement (RII) project will enable Louisiana researchers in many disciplines to participate in worldwide grid-computing — a network of many separate computers addressing large-scale computational problems.

The hardware for creating a thriving environment for research efforts across the State is already in place: the Louisiana Optical Network Initiative (LONI). This fiber optic network links supercomputers at the State's major universities and research centers to the National LambdaRail, one of the most advanced computing infrastructures in the nation.

The RII project is guided by the concept that cyberinfrastructure development must be guided by scientific questions and, conversely, the scientific strategies must include advanced cyberinfrastructure.

The RII CyberTools component specifically targets the project's two key research themes: Sensors and Systems, and Simulation and Modeling. Their selection was based on the significant expertise of the participating researchers, as well as the considerable opportunities awaiting cyberinfrastructure that enables molecular and fluid flow simulations and capabilities well beyond those now available.

The Science Drivers were highlighted in the November issue; highlights of the CyberTools component follow.

CyberTools Work Packages

Four CyberTools Work Packages (WPs) address the scientific priorities of the Science Drivers' common needs in theory, methodology, in the development of well-defined computational plans, and in the cyberinfrastructure required to advance them in a 21st century computing environment.

WP 1: Scheduling and Data Services

The efficient management, retrieval, and mining of distributed, heterogeneous data is a daunting problem, critical to many applications.

Dr. Donald Gaver, Chair, Tulane Biomedical Engineering Department, and one of the three Science Driver team leaders, addressing the RII project kick-off meeting.

The complexity and heterogeneity of a computational process in which different parts of a program are run simultaneously on two or more computers communicating with each other over a network, for example, require a robust layer of information and scheduling services that don't break down easily or are not wholly affected by an application failure.

Data Archival & Retrieval Services Services to automatically archive data directly from simulations and experiments and to efficiently and reliably retrieve them are being created for all of the science projects.

Scheduling Services Enhanced scheduling services will support automated, on-demand simulations for hurricane/surge forecasting; simultaneous computational fluid mechanics to recreate the real world behaviors of liquids and gases in a virtual environment; molecular dynamics simulations; and coupled simulation-visualization processes.

Welcoming researchers at the project's kick-off meeting is Dr. Michael Khonsari, RII Project Director.

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CyberTools *Continued from pg 1*

High Availability Uninterrupted availability for mission-critical applications and services will be ensured through a system that addresses reliability, availability, and serviceability issues by automatically handling software and hardware faults. Novel mechanisms such as self-healing, failure detection and recovery will also be incorporated.

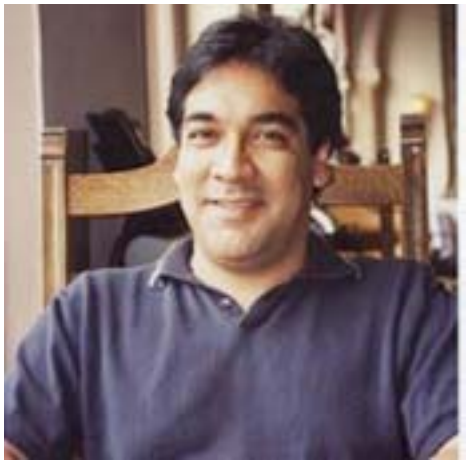
Metadata Extraction The RII project will be generating voluminous and complex data. Definitive lists of instructions for data mining and metadata descriptions — data describing anything from an individual datum to data with multiple content items — are thus being developed.

WP 2: Information Services and Portals Reliable, up-to-date information is vital for developing and implementing the various scientific applications. Information services are being developed for discovering, monitoring, and providing information about computer, network, and data resources, and for running applications and experiments.

The deployment and reuse of complex software and new grid technologies are being simplified and a set of protocols, models, encoding rules, and tools enabling scientists to interact in a heterogeneous information services infrastructure is being developed.

Application-specific, point-of-access sites are being designed for each group of collaborators, as are simplified interfaces enabling non-expert users to link to resources and services, collect information, monitor jobs, and support collaborations.

WP 3: Visualization Services Grid and virtual environments add complexity to visualization, a key component of all projects, making its integration daunting. This team will address that issue by integrating, leveraging and building visualization activities that will help drive LONI-based research as well as the educational use of Louisiana's visualization infrastructure.



Dr. Ricardo Cortez, Director, Tulane University Center for Computational Science, and one of the three RII Science Driver team leaders.

Data and visualization integration A large fraction of visualization efforts is consumed helping scientists migrate their data into proper formats. An architecture enabling front-end visualization is being developed and integrated into the high-definition streaming visualization service (see below) to enable scientists to share and discuss their results over LONI.

High definition streaming visualization The focus is on providing visualization services that enable applications to scale from desktops to the most advanced systems with minimal effort.

WP 4: Application Services and Toolkits This, the central WP, supports the development of codes for all projects. Without modification, traditional application software run in a modern grid environment would be blind to the advanced computer, data, network, and visualization services found in LONI's modern cyberinfrastructure environment.

Exploiting the LONI computing environment and future petascale systems — which make mathematic calculations at a sizzling 1,000-trillion operations per second — this WP team will create a foundation for computing services for virtually every discipline across the State for decades to come.

A particular focus will be on a complex system that simulates and makes predictions regarding how physical/artificial/social entities will change and continuously adjusts the simulations, influencing how and where future data will be gathered in order to focus on areas of uncertainty.

Computational Fluid Dynamics & Molecular Dynamics Toolkits All of the science and engineering projects make use of computational fluid dynamic (CFD) techniques to recreate the real-world behaviors of liquids and gasses in a virtual environment and most use molecular dynamics (MD), a computer simulation of the motion of atoms.

Teams will research and develop discipline-specific abstractions, creating advanced CFD and MD toolkits, bringing together researchers across the State and creating new capabilities not currently available.

"By the project's end, the CyberTools team will have created production-ready and demonstration-example applications in areas of fluid flow simulations, storm-surge modeling, hurricane simulation, airplane design, biofluids, and bioinformatics," says Dr. Khonsari, RII Principal Investigator, Louisiana EPSCoR Project Director, and Board of Regents Associate Commissioner for Sponsored Programs Research and Development.

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