NSF Launches Distributed Data Analysis of Neutron Scattering

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The DANSE project will integrate new materials theory with high-performance computing, using data from facilities such as the Department of Energy's new Spallation Neutron Source in Oak Ridge, Tenn. In this image, Rick Martineau of Los Alamos National Laboratory gives a final inspection to a componant of the SNS prior to shipment. Credit: Leroy N. Sanchez, Los Alamos National Laboratory

The National Science Foundation (NSF) has awarded nearly $12 million to the California Institute of Technology for computer software to analyze neutron-scattering experiments. The work could show how to design new materials for a huge variety of applications in transportation, construction, electronics and space exploration.

The five-year Distributed Data Analysis for Neutron Scattering Experiments (DANSE) project is led by Brent Fultz, a professor of

materials science and applied physics at Caltech, with co-principal investigators Michael A. G. Aivazis of the Center for Advanced Computing Research at Caltech, and Ian S. Anderson of the Spallation Neutron Source (SNS) in Oak Ridge, Tenn.

Neutron scattering is a method of analyzing the stability of materials, molecules, and condensed matter at various temperatures and pressures by looking at the positions and motions of the atoms that making up the materials. According to Fultz, the research will find the principles behind how atoms can be combined to form stable materials and will eventually show how new materials could be optimized for characteristics such as mechanical strength, electrical conductivity, energy storage and corrosion resistance.

The low intensities of today's neutron sources have been impaired many neutron-scattering measurements. That will change in 2008 as the SNS, constructed by the Department of Energy at a cost of $1.4 billion, begins to operate at high power. The unprecedented quality of data from the SNS will allow a deeper understanding of atom interactions, for example, and will require better methods for interpreting the measurements.

NSF's DANSE project arises from recent developments in computing, materials theory and the new experimental facilities at the SNS. The project integrates new materials theory with high-performance computing to push the science of the SNS and other neutron facilities to a higher level of sophistication. The project will also extend a software framework developed at Caltech to include distributed computing on today's networked computing hardware.

The DANSE project is centered at Caltech where its software technology effort, neutron-scattering research, and project administration will be conducted. The grant includes smaller awards to

four other universities for subfields of neutron-scattering research: neutron diffraction (Simon Billinge, Michigan State University); engineering diffraction (Erstan Ustundag, Iowa State University); small-angle scattering (Paul Butler, University of Tennessee); and reflectometry (Paul Kienzle, University of Maryland). All these different subfields need advanced scientific computing for comparing experimental data to underlying physical models or simulations, and all will benefit from a shared development effort. DANSE will develop new methods for doing neutron-scattering research in these subfields.

The NSF funding will also support an outreach effort in teacher education, which is being created by Iowa State University.

Source: NSF