A NEW SPECIALIZED SYSTEM FOR BIOMOLECULAR RESEARCH

A $2.7M GRANT FROM THE NIH WILL ALLOW THE NATIONAL RESOURCE FOR BIOMEDICAL SUPERCOMPUTING AT PSC TO PROVIDE U.S. BIOMEDICAL RESEARCHERS WITH ACCESS TO A NOVEL SPECIAL-PURPOSE SUPERCOMPUTER FOR BIOMOLECULAR SIMULATION, MADE AVAILABLE WITHOUT COST BY D. E. SHAW RESEARCH.

Anton was designed to dramatically increase the speed of “molecular dynamics” (MD) simulations compared with the previous state-of-the-art, allowing biomedical researchers to understand the motions and interactions of proteins and other biologically important molecules over much longer time periods than have previously been accessible to computational study. The machine, called Anton, will be made available without cost by DESRES for non-commercial research by universities and other non-profit institutions.

The National Institute of General Medical Sciences (NIGMS), part of the National Institutes of Health, has awarded a two-year, $2.7 million grant to the National Resource for Biomedical Supercomputing (NRBSC) at PSC to host a specialized supercomputer for biomolecular simulation designed by D. E. Shaw Research (DESRES). The machine, called Anton, was designed to dramatically increase the speed of molecular dynamics (MD) simulations compared with previous methods. Anton is intended to make accessible to computational study a much larger dataset of biological information.

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PSC AND TERAGRID

PSC is actively involved in TeraGrid leadership. Scientific director Ralph Kunzler oversees PSC contributions to the integrating efforts of the national Grid Infrastructure Group that guides TeraGrid. Co-scientific director Michael Levine is PSC’s representative to the TeraGrid Forum—TeraGrid’s principal decision-making group.

Other PSC staff with TeraGrid leadership roles include Sergiu Sanielevici, Area Director for User Support and Jim Mantellier, head of PSC’s security, who chairs the TeraGrid Security Working Group. Laura McGinnis plays a lead role in TeraGrid education, outreach and training (EOT) activities, PSC director of systems and operations. J. Ray Scott, leads the TeraGrid effort in data management, and PSC director of strategic applications, Nick Nystrom, leads the TeraGrid Extreme Scalability Working Group, which fosters planning to meet the challenges of deploying extreme-scale resources into the TeraGrid.

PSC staff members serve on all of TeraGrid’s working groups.

The TeraGrid is the world’s most comprehensive distributed cyberinfrastructure for open scientific research. As a major partner in this National Science Foundation program, PSC helps shape the vision and progress of the TeraGrid.

The Teragrid Resource Providers

Indiana University
Louisiana Optical Network Initiative
National Center for Supercomputing Applications
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Pittsburgh Supercomputing Center
Purdue University
San Diego Supercomputer Center
Texas Advanced Computing Center
The University of Chicago/Argonne National Laboratory

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PSC staff who work contributes to the TeraGrid

Include 3 to 4 scientists: David Moses, PSC executive director; Laura McGinni, PSC manager of education and training; Sergiu Sanielevici, PSC director of scientific applications and user support; J. Ray Scott, PSC director of systems and operations.

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