SURAgrid Update – February 2010

NEWS

- - SURAgrid Spring 2010 All Hands Meeting Update - -

Meeting Agenda -
The Spring All Hands Meeting is scheduled for March 24 – 26 in Washington, DC. The first day of the meeting, Wednesday March 24, will be a joint session with CASC and the EDUCAUSE Committee on Cyberinfrastructure, and will be held at the Westin Arlington Gateway Hotel. Topics for the joint session include:

(1) The recommendations from the August 2008 CASC/EDUCAUSE CI workshop (http://www.casc.org/papers/CASC-CCI_Workshop_Report_and_Recommendations.pdf);
(2) The NSF Dear Colleague Letter on infusing CI throughout the agency directorate (http://www.nsf.gov/dir/index.jsp?org=OC);
(3) And presentations from campuses on their CI initiatives and activities.

The sessions on Thursday March 25 and Friday March 26 will be held at the SURA offices located at 1201 New York Avenue, NW, Washington, DC. The SURAgrid meeting will be focused on the work to improve and enhance SURAgrid operations and user services. The SURAgrid meeting will end no later than noon on Friday March 26.

Additional information on the agenda will be provided via email updates to the SURAgrid listserv.

Meeting Lodging -
The CASC room block is available to SURAgrid meeting participants at a government rate of $226 for the nights of Sunday, March 21 through Thursday, March 25. Reservations can be made at http://www.starwoodmeeting.com/Book/CASC0310.

There is a SURA rate of $199 at the Morrison Clark Hotel, 1015 L St NW, Washington, DC if rooms are available. SURA is not holding a block of rooms due to limited usage of the room block at prior meetings. Other hotels near the SURA offices include:

- Four Points by Sheraton, 1201 K St NW, Washington, DC
- Hilton Garden Inn, 815 14th St NW, Washington, DC
- Holiday Inn, 1501 Rhode Island Ave NW, Washington, DC
- Doubletree Hotel, 1515 Rhode Island Avenue NW, Washington, DC

SURA offices and the Westin Gateway are accessible via metrorail from the Americana Hotel in Arlington, which has room rates under $100 per night. http://www.americanahotel.com

- - Building Campus CI Capacity at Norfolk State University - -

Contributed by: Eduardo Socolovsky, Norfolk State University

In December 2009, a very successful High Performance – High Throughput Computing (HPC-HTC) workshop was held at the Norfolk State University (NSU) Virtualization and Collaboration Center. The workshop was co-sponsored by the Center for Biotechnology (CBBS) of Norfolk State University (NSU), the High Performance Computing Center (HPCC) of Texas Tech University (TTU), and SURAgrid. Led by Jerry Perez of TTU, the workshop resulted in the establishment of a campus grid at NSU using Condor middleware.

Norfolk State University's CBBS has a growing drug discovery research program that is beginning to demand increasingly more powerful and robust computational, data storage, and visualization resources. When using standard computational resources, computing time for bioinformatics tasks supporting drug

discovery can be extraordinarily long, and in many cases require extremely large storage capacity. For some tasks, the feasibility of the computation would be challenged without HPC-HTC.

Two example applications are Virtual Screening and Micro-Array Data Analysis. Virtual Screening of (hundreds of) thousands of small compound drug candidates (often called ligands) can take weeks or months on a standard Xeon workstation. Instead, the time can be reduced to a few hours on a grid by docking many ligands simultaneously, each ligand in an independent processor. Another example, from Micro-Array Data Analysis, is testing the stability of the data clusters that identify the expressed genes. This testing is done by taking hundreds of samples from the original micro-array data set and re-clustering these samples with the exact same method. Clustering itself is compute intensive, and on a grid many samples can be clustered simultaneously, each sample in an independent processor.

The partnership between SURA and the CBBS started with the SURA-Microsoft Cluster Computing project, that involved installing and using BioHPC, a bioinformatics software environment developed by Cornell University for Microsoft's HPC2008. Attracted by SURAgrid's vision to bring Grid technology to the level of seamless shared campus to campus cyber-infrastructure that orchestrates access to a rich set of distributed middle scale capabilities in order to meet diverse users' needs, NSU CBBS joined SURAgrid. NSU's collaboration with SURAgrid and its members has grown into other areas of cyber-infrastructure, exploration of collaborative funding opportunities, and outreach to broaden participation in CI and includes the CBBS being represented on SURAgrid's Governance Committee. This most recent HPC-HTC workshop is just one additional way in which NSU CBBS has been able to leverage its participation in SURAgrid.

UPCOMING EVENTS

- Mar 8 – 11, Open Science Grid All Hands Meeting, Fermilab, Batavia, IL
- Mar 22 – 24, Coalition for Academic Scientific Computing, Arlington, VA
- Mar 24 – 26, SURAgrid All Hands Meeting, Washington, DC
- Apr 26-28, Spring Internet2 Member Meeting, Arlington, VA

All issues of SURAgrid update can be found at http://sura.org/programs/sura_grid_communications.html. Please submit comments and contributions for inclusion to Linda Akli at akli@sura.org.